

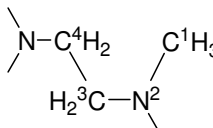
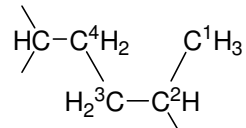
# First Principles Study of Ignition Mechanism of Hypergolic Bipropellant: N,N,N',N'-tetramethylethylenediamine (TMEDA), N,N,N',N'-Tetramethylmethylenediamine (TMMDA) and Nitric Acid

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## Supporting Information:

This material includes two sections: 1. The barriers and TS geometries of H-abstraction on TMEDA and 2,5-dimethyl-hexane with different NO<sub>2</sub> orientations. 2. All geometries of TS and intermediate in all schemes.

### 1. The barriers of H-abstraction on TMEDA and 2,5-dimethyl-hexane

	TMEDA	2,5-dimethyl-hexane
Barrier Height (kcal/mol)		
C <sup>1</sup> -cis-HONO	8.3	24.4
C <sup>1</sup> -trans-HONO	15.6	30.2
C <sup>1</sup> -HNO <sub>2</sub>	11.4	26.3
C <sup>3</sup> -cis-HONO	8.0	20.9
C <sup>3</sup> -trans-HONO	16.3	27.2
C <sup>3</sup> -HNO <sub>2</sub>	11.5	21.6

TS for H-abstraction on 2,5-dimethyl-hexane:

C<sup>1</sup>-cis-HONO E=-520.88845754848

C1	2.8462854347	7.6616922785	12.6147524800
C2	3.2123083897	9.1493001493	12.5144990309
H3	2.4544897030	9.7712922800	13.0038126391
H4	3.2870507152	9.4726353810	11.4722543893
H5	4.1714356826	9.3546823468	12.9986075695
C6	2.8227244380	7.2149026420	14.0837009776
H7	2.0441274928	7.7504407080	14.6386790815
H8	3.7795389600	7.4262627695	14.5696716115
H9	2.6330671274	6.1442013235	14.1901989520
C10	1.5132414594	7.3862177483	11.8891766644

H11	1.5596147055	7.8666185964	10.9058750934
H12	0.7031784768	7.8848228694	12.4401950486
C13	-0.2084360700	5.6082523181	11.0849986476
C14	-0.4768733800	4.0992377456	11.0194721128
H15	0.2274993673	3.6122805145	10.3413919783
H16	-0.3729651621	3.6431770046	12.0076776867
H17	-1.4894030447	3.8933534688	10.6607963068
C18	-0.4415793008	6.2872100836	9.7586488193
H19	0.6956409367	6.1718030002	8.9026557923
H20	-1.2156687976	5.8563631809	9.1240919190
H21	-0.4540541236	7.3770685290	9.7615050559
C22	1.1754354062	5.9016481217	11.7096240577
H23	1.2051278162	5.3948332625	12.6789978604
H24	1.9442352146	5.4232897712	11.0904822566
N26	2.1674146239	5.1704199540	7.8648048410
O27	1.5886316774	6.3117490720	8.1543974294
O28	1.7539698711	4.1819381050	8.3933242166
H28	3.6290416786	7.0893861581	12.0986550400
H29	-0.9578267146	6.0518357119	11.7669888888

C<sup>1</sup>-trans-HONO E= -520.87897183748

C1	2.7737117501	7.7180423999	12.5388752290
C2	3.0661009998	9.2249556986	12.5610656229
H3	2.3242401553	9.7575655978	13.1665645888
H4	3.0425663416	9.6502774356	11.5537211186
H5	4.0515703213	9.4308941234	12.9886492836
C6	2.8863070943	7.1288441158	13.9522289877
H7	2.1302664599	7.5644993376	14.6153178564
H8	3.8678572086	7.3424940201	14.3849645838
H9	2.7553869418	6.0440914331	13.9622294254
C10	1.4019391287	7.4481225148	11.8877028448
H11	1.3615130942	8.0135662017	10.9510778606
H12	0.6155363638	7.8605984232	12.5356890888
C13	-0.2793343104	5.6772442983	10.9922642737
C14	-0.5054724157	4.1668695860	10.8368100571
H15	0.2133536300	3.7388190360	10.1316237351
H16	-0.3826953517	3.6523814386	11.7933119452
H17	-1.5108533911	3.9498653193	10.4651444882
C18	-0.5429214293	6.4123199483	9.6933454858
H19	0.3458248791	6.1160281347	8.9005571960
H20	-1.4456203309	6.0962394093	9.1662911827
H21	-0.4678297241	7.4987861108	9.7402046559
C22	1.1089090332	5.9708224748	11.5995655167
H23	1.1903207085	5.3901125840	12.5235961312
H24	1.8733325630	5.5754688386	10.9196017462
N26	2.0929903699	7.0200008835	8.0727814425
O27	1.3645465133	5.8629676005	8.0588139678
O28	3.0260180169	6.9360127495	7.3415357292
H28	3.5367403838	7.2393218074	11.9103040988
H29	-1.0345277853	6.0611038702	11.7008318661

C<sup>1</sup>-HNO<sub>2</sub> E=-520.88704766870

C1	2.7476577006	8.2985880212	12.6869638769
C2	2.5802255393	9.1493596729	13.9535887309
H3	2.1463426215	8.5569127361	14.7666273697
H4	1.9218054630	10.0051089016	13.7769997910
H5	3.5430576623	9.5337786773	14.3022098489
C6	3.7209968414	7.1385632227	12.9413775755
H7	3.3158344395	6.4488727193	13.6901959721
H8	4.6788129108	7.5099399374	13.3169323857
H9	3.9246610682	6.5628761495	12.0356006235
C10	1.3751328469	7.8160133613	12.1783160759
H11	0.7090598504	8.6852445342	12.0999297984
H12	0.9353897296	7.1599414022	12.9392548884
C13	0.0198787001	6.7835194370	10.2283016397
C14	-0.8011205745	5.8081077486	11.0897032124
H15	-0.2689732137	4.8605578781	11.2119648571
H16	-0.9933625434	6.2172877633	12.0829996514
H17	-1.7694254650	5.5984397284	10.6263555806
C18	0.1251820070	6.3087664498	8.8054241300
H19	0.9168384656	4.9545960556	8.8338194425
H20	-0.7772614631	5.9297255231	8.3273912081
H21	0.7938468939	6.8492890015	8.1364431633
C22	1.4106421702	7.0986837788	10.8230782640
H23	1.9703847802	6.1616986071	10.9077044943
H24	1.9565228694	7.7273218808	10.1078401474
N26	1.5008886375	3.9463291143	8.8405271174
O27	1.6943262955	3.4395981443	7.7566638412
O28	1.8409202917	3.5330873951	9.9327691038
H28	3.1833714064	8.9399192787	11.9082496179
H29	-0.5385926003	7.7375063741	10.1858738239

C<sup>3</sup>-cis-HONO E= -520.89321281509

C1	3.1062647286	7.4536771289	13.2348565015
C2	3.2832505341	8.9726264846	13.3668000894
H3	2.4596309944	9.4156370810	13.9375070882
H4	3.3103404796	9.4573202471	12.3869638087
H5	4.2141829349	9.2167386409	13.8856802599
C6	3.1536036203	6.7845600317	14.6157495341
H7	2.3316862547	7.1384656114	15.2480308236
H8	4.0905983233	7.0202667518	15.1277476059
H9	3.0828229531	5.6955838664	14.5548346811
C10	1.8002371263	7.1377121587	12.4759918647
H11	1.7368541091	7.7828201415	11.5924499747
H12	0.9467213762	7.4293838133	13.1119689568
C13	0.2804681527	5.3024220490	11.4165037273
C14	0.0912537495	3.7809634829	11.3620552292
H15	0.8435544048	3.3212307201	10.7178229207
H16	0.1735634822	3.3362261437	12.3581661692
H17	-0.8957630009	3.5284595853	10.9649662688
C18	0.0542744612	5.9418283282	10.0350126670
H19	0.7586118944	5.5345653764	9.3049479255

H20	-0.9561491264	5.7257854770	9.6786121056
H21	0.1722294913	7.0275708121	10.0582866528
C22	1.5990651911	5.6945556571	12.0637711957
H23	1.9478312173	4.9670900604	12.8005753134
H24	2.6327850753	5.5365138912	11.1194102043
N26	3.7882176845	4.7099262793	9.5701131990
O27	3.6283970447	5.6574116039	10.4587768526
O28	2.9430084825	3.8681741001	9.4830890038
H28	-0.4960472540	5.7086204018	12.0884538347
H29	3.9415252390	7.0698951398	12.6381411266

C<sup>3</sup>-trans-HONO E= -520.88380633442

C1	3.1442887569	7.2026098534	13.1343309582
C2	3.5177739245	8.6860299550	13.0121492625
H3	2.7122791984	9.3254282778	13.3901187954
H4	3.7058017488	8.9628716652	11.9712231986
H5	4.4190598131	8.9140737809	13.5879469484
C6	2.9777501839	6.8055882563	14.6080402151
H7	2.1748546056	7.3850843274	15.0770964083
H8	3.8964649690	6.9979684916	15.1688566941
H9	2.7386752735	5.7456964930	14.7298241030
C10	1.8830608504	6.8965559701	12.3007795463
H11	1.9608939620	7.4083041868	11.3362626600
H12	1.0050996917	7.3346053657	12.8029480184
C13	0.2771299185	5.0139165050	11.4438668378
C14	0.1858214513	3.4904502482	11.2775447913
H15	0.9245234577	3.1346515670	10.5534561345
H16	0.3658232843	2.9730255300	12.2242299717
H17	-0.8039705204	3.1970603296	10.9181394265
C18	-0.0386219271	5.7348623413	10.1254107227
H19	0.7029987890	5.4871810770	9.3608132013
H20	-1.0187961807	5.4286832649	9.7507573514
H21	-0.0530596233	6.8205571031	10.2417375437
C22	1.6125583562	5.4231943288	12.0619523130
H23	1.8519011191	4.8002637628	12.9303618159
H24	2.4717299067	5.0480597243	11.2867765119
N26	3.7348995288	5.8652767553	9.7423923600
O27	3.4723902944	4.7058626477	10.3796043595
O28	4.5912917241	5.7460823359	8.9205187558
H28	3.9694617231	6.6146927503	12.7138789352
H29	-0.4859440178	5.3161821416	12.1805344856

C<sup>3</sup>-HNO<sub>2</sub> E= -520.89337912712

C1	3.1020646407	7.3879387405	13.2301224548
C2	3.4244967999	8.8876137939	13.1853641868
H3	2.6083115810	9.4780722387	13.6167358393
H4	3.5811701825	9.2311403744	12.1589120876
H5	4.3313628487	9.1115230245	13.7537304508
C6	2.9745876328	6.9072767784	14.6825233484
H7	2.1631216630	7.4352160835	15.1960136574
H8	3.8975035962	7.0976432554	15.2370197487

H9	2.7692875380	5.8356042342	14.7511086833
C10	1.8298031947	7.0897806690	12.4083974743
H11	1.8789265740	7.6411287363	11.4610963447
H12	0.9575146130	7.5134030229	12.9366161882
C13	0.2327449870	5.1990246907	11.5405060228
C14	0.1728115964	3.6778399229	11.3305853370
H15	0.8894813041	3.3620143953	10.5677370496
H16	0.3979299567	3.1397920529	12.2561218344
H17	-0.8232503101	3.3719559132	11.0002745084
C18	-0.1425538609	5.9517901993	10.2521418192
H19	0.5657080954	5.7257898506	9.4499184808
H20	-1.1352881771	5.6462831498	9.9120131887
H21	-0.1628967026	7.0340115252	10.3990810452
C22	1.5591425003	5.6305169577	12.1345846951
H23	1.9422552452	4.9408406451	12.8899474414
H24	2.5901916318	5.2873307246	11.0710035183
N26	3.4212391587	5.0727734509	10.2388089170
O27	4.5135924041	5.5634506843	10.4399037729
O28	3.0757395845	4.3959813385	9.2905964939
H28	3.9345424989	6.8529099187	12.7587665561
H29	-0.5254174647	5.4587958281	12.3011199646

TS for H-abstraction on TMEDA

C<sup>1</sup>-trans-HONO E= -552.94608040044

N1	2.6873031573	7.4083759281	12.5509752659
C2	3.3899464946	8.6313719726	12.1755031914
H3	2.8284457479	9.5500912552	12.4267194912
H4	3.5861604247	8.6309615170	11.1018161670
H5	4.3502791677	8.6723636245	12.6957618000
C6	2.4810586717	7.3284656163	13.9900815025
H7	1.8523987434	8.1516688513	14.3793230904
H8	3.4446639839	7.3652124088	14.5039503452
H9	2.0019650077	6.3840037707	14.2591772333
C10	1.4595554669	7.2071940564	11.7862245316
H11	1.5763678217	7.6942438538	10.8171009570
H12	0.5797549031	7.6553622868	12.2822347038
N13	-0.0201667077	5.3686962012	10.8805772706
C14	-0.2766873448	3.9425032239	10.7646962535
H15	0.4126615316	3.4686543625	10.0509792003
H16	-0.1451514454	3.4653755810	11.7378092935
H17	-1.2992633179	3.7764053355	10.4241136764
C18	-0.4972621466	6.1949519784	9.8460242698
H19	0.2619891065	6.2014547904	8.9242618154
H20	-1.4578658094	5.8448133886	9.4669673625
H21	-0.5434255151	7.2458123509	10.1335270868
C22	1.2320430352	5.7094289220	11.5586060605
H23	1.2371569748	5.1765611400	12.5135658533
H24	2.0782902046	5.3220846933	10.9724328170
N26	1.9482179583	7.4546699267	8.3244281382
O27	1.3225454904	6.3915789718	7.8893723161
O28	2.8815057124	7.8168740355	7.6482143216

C<sup>1</sup>-HNO<sub>2</sub> E= -552.95266430508

N1	2.7064847548	8.1034306808	12.8427245703
C2	2.6574229669	9.3816435456	13.5422011869
H3	2.0016006874	9.3657854263	14.4330089973
H4	2.2985440434	10.1623390642	12.8675503082
H5	3.6626062540	9.6570868694	13.8706045501
C6	3.2782576803	7.0654736104	13.6935429378
H7	2.6678923479	6.8694930821	14.5956029602
H8	4.2761792655	7.3685628076	14.0183377478
H9	3.3834921771	6.1285299622	13.1445060816
C10	1.4057880104	7.7322533011	12.2936271663
H11	0.9280080610	8.6334574333	11.9008313054
H12	0.7318060539	7.3292363178	13.0728003565
N13	0.2460905975	6.3836943659	10.5519180264
C14	-0.5263517027	5.3669731828	11.2584305883
H15	-0.0851981314	4.3722720147	11.1195703952
H16	-0.5563853316	5.5947536709	12.3245167616
H17	-1.5501401394	5.3593509951	10.8806052002
C18	0.0869814813	6.4708073058	9.1740478307
H19	0.7815672345	5.3141423516	8.5845232972
H20	-0.9406823669	6.3356905723	8.8385273924
H21	0.5950731460	7.3201545556	8.7207967722
C22	1.5435009116	6.7353564747	11.1330272070
H23	2.0560474105	5.8196804069	11.4465852655
H24	2.1588649034	7.1959830775	10.3595468554
N26	1.4226568903	4.2811710201	8.3243875673
O27	1.5717089899	3.9429318400	7.1668934324
O28	1.8538089298	3.6983669266	9.3128553604

C<sup>3</sup>-trans-HONO E= -552.94489528078

N1	3.0250148637	7.3630754972	13.3897974130
C2	3.5617275889	8.7134672557	13.2809918113
H3	2.8208585350	9.4995158213	13.5196936796
H4	3.9339773432	8.8835236608	12.2688520277
H5	4.4026800164	8.8260001483	13.9694073326
C6	2.6320103245	7.0513886415	14.7569183844
H7	1.8273050096	7.7116906319	15.1324660444
H8	3.4939188453	7.1526437024	15.4203013211
H9	2.2807712809	6.0196965935	14.8298892438
C10	1.9671190508	7.0921175417	12.4249493148
H11	2.1506951930	7.7010921999	11.5371264754
H12	0.9708094513	7.3753670299	12.8147411524
N13	0.8167069539	5.1161741786	11.3856291091
C14	0.6261203056	3.6756030374	11.2990368622
H15	1.0533740633	3.2682133156	10.3768662701
H16	1.1060557567	3.1922066914	12.1501958071
H17	-0.4439424992	3.4470456050	11.3215507532
C18	0.1219528291	5.9046022841	10.3772194842
H19	0.5984578306	5.8103107280	9.3958532936
H20	-0.9099546386	5.5529364929	10.3001612582

H21	0.1048011058	6.9555914838	10.6617807517
C22	1.9745458864	5.6081484863	12.0269573208
H23	2.2159111361	4.9670364697	12.8783569087
H24	2.9076289988	5.4887575142	11.3104320967
N26	3.2652687931	4.8474458323	9.2774588035
O27	3.9683778769	5.3816932037	10.2258192873
O28	3.8403349965	4.6249664945	8.2352985528

C<sup>3</sup>-HNO<sub>2</sub> E= -552.95214953727

N1	2.8891311644	7.1477020002	13.3341623836
C2	3.6170106011	8.3784535877	13.0523541236
H3	3.0273842467	9.2932895133	13.2500603028
H4	3.9356603756	8.3787529187	12.0086317799
H5	4.5135762753	8.4176239153	13.6761730426
C6	2.5696638703	7.0019750320	14.7463667614
H7	1.9064735800	7.8037917068	15.1232750009
H8	3.4885751861	7.0140725966	15.3374720739
H9	2.0726743058	6.0450636162	14.9253694975
C10	1.7260084329	6.9499609538	12.4736892413
H11	1.8599734218	7.5508507497	11.5695887385
H12	0.7931810625	7.3092802141	12.9514024673
N13	0.4152258879	5.0071442467	11.5402792977
C14	0.3098156785	3.5633565836	11.3519380418
H15	0.8959019586	3.2210064080	10.4888921075
H16	0.6749276799	3.0529934033	12.2444945053
H17	-0.7370362336	3.2912184300	11.2008667481
C18	-0.2320915776	5.7966696138	10.5004464900
H19	0.2871740839	5.7098012620	9.5340316930
H20	-1.2578475943	5.4462752028	10.3687371775
H21	-0.2656997476	6.8477354691	10.7849495376
C22	1.6019695868	5.4771335906	12.1060977656
H23	1.9795834813	4.8040683632	12.8755245300
H24	2.6626539769	5.3741188999	11.1056489991
N26	3.4515044311	5.3750289946	10.1408985475
O27	4.1030553982	6.3871130649	9.9437930023
O28	3.4294298489	4.3811819288	9.4318132908

2. Geometries of TS and intermediate shown in Scheme 1 and Scheme 2.

TMEDA E=-347.84108634136

N1	0.5367749740	1.6005457016	0.8590594816
C2	-0.2065641528	2.7804307518	1.2804132250
H3	-0.8358873480	2.6042145810	2.1737792207
H4	-0.8551592710	3.1216902219	0.4699993136
H5	0.4899311340	3.5894421998	1.5161258284
C6	1.4829144534	1.1926924897	1.8897844679
H7	0.9858309433	0.8809527163	2.8285485885
H8	2.1528099498	2.0245686010	2.1210507396
H9	2.1002357000	0.3626569010	1.5426362210
C10	-0.3534509795	0.5165245965	0.4432654293
H11	-1.1730304242	0.9696582707	-0.1196289637

H12	-0.8084821078	-0.0061242229	1.3045591994
N13	-0.5367749740	-1.6005457016	-0.8590594816
C14	0.2065641528	-2.7804307518	-1.2804132250
H15	0.8358873480	-2.6042145810	-2.1737792207
H16	0.8551592710	-3.1216902219	-0.4699993136
H17	-0.4899311340	-3.5894421998	-1.5161258284
C18	-1.4829144534	-1.1926924897	-1.8897844679
H19	-0.9858309433	-0.8809527163	-2.8285485885
H20	-2.1528099498	-2.0245686010	-2.1210507396
H21	-2.1002357000	-0.3626569010	-1.5426362210
C22	0.3534509795	-0.5165245965	-0.4432654293
H23	1.1730304242	-0.9696582707	0.1196289637
H24	0.8084821078	0.0061242229	-1.3045591994

INT1: E=-347.18545072851

N1	2.7046462273	7.5007636297	12.4680091136
C2	2.9799472996	8.9311737680	12.4322743564
H3	2.2713571675	9.5270271994	13.0386413688
H4	2.9342486567	9.2934623699	11.4025843416
H5	3.9876413555	9.1212836026	12.8110752762
C6	2.8568282262	6.9772513000	13.8195837185
H7	2.1253659274	7.4071966792	14.5308392733
H8	3.8603853081	7.2027382099	14.1884269280
H9	2.7417918389	5.8919030812	13.8299381105
C10	1.4064499413	7.1824306187	11.8787736059
H11	1.2883495473	7.7923219748	10.9799196188
H12	0.5657306706	7.4416503114	12.5497455230
N13	0.0272375539	5.4348289975	10.7852637676
C14	-0.7143324222	4.2584510797	11.2095241832
H15	-0.2350241257	3.3188361241	10.8923362227
H16	-0.8138492807	4.2511662876	12.2971985664
H17	-1.7171132938	4.2881362858	10.7774335525
C18	-0.0643868295	5.7875399589	9.4485086478
H20	-1.0197126038	5.6301414546	8.9645145792
H21	0.5681119690	6.5934303294	9.1028756356
C22	1.2870785649	5.7048386737	11.4743589565
H23	1.3252868955	5.0699602420	12.3614079514
H24	2.1475814743	5.4382110190	10.8458802205

HONO E= -205.76177088913

H19	0.8859488087	1.5742679777	0.0000000000
N26	0.4437989608	-0.2654386209	0.0000000000
O27	0.0373546669	1.1085236860	0.0000000000
O28	-0.4817103416	-0.9753332297	0.0000000000

INT2: E=-347.19153181016

N1	2.7971042181	7.2953159229	13.2809449668
C2	3.2729632741	8.6501546347	13.4962160372
H3	2.4550331057	9.3889639494	13.4803808381
H4	3.9953736885	8.9175805932	12.7228973180
H5	3.7709836845	8.7142700863	14.4672018077
C6	1.9898697198	6.7772931575	14.3786252258



H7	1.1174591153	7.4225449612	14.5738265975
H8	2.5930558611	6.7300051327	15.2901343497
H9	1.6133052210	5.7878367918	14.1316143672
C10	2.4974356415	6.9332657690	11.9726604434
H11	3.0007611804	7.5342932423	11.2251485263
N13	0.7692882906	5.1059475233	11.9177681486
C14	0.5908460064	3.6789383556	11.6976624908
H15	0.7434465142	3.3807621117	10.6419752322
H16	1.2977806823	3.1144617104	12.3120006773
H17	-0.4211199081	3.3831833136	11.9864003767
C18	-0.2112299109	5.8811301607	11.1703389012
H19	-0.1470355653	5.7101783173	10.0778128989
H20	-1.2201010870	5.6154252591	11.4971418876
H21	-0.0514728144	6.9448400264	11.3556265968
C22	2.1545092336	5.5209421040	11.6158756069
H23	2.8093540938	4.8200007269	12.1567710476
H24	2.3721544881	5.3841262117	10.5395770170

INT3: E=-379.08364317087

N13	0.3402260787	5.0808170784	11.9538532930
C14	0.0652537310	5.2891929718	10.5351696532
H15	-0.7519168903	6.0067442087	10.4276301803
H16	0.9493214289	5.7084806314	10.0489942212
H17	-0.2132563624	4.3647461226	10.0078086533
C18	-0.8186898801	4.6127546112	12.7054215865
H19	-1.6350558094	5.3302899869	12.5933326890
H20	-1.1828605696	3.6268605156	12.3758710993
H21	-0.5679061263	4.5477920188	13.7664166907
C22	1.5502652121	4.4003233837	12.2350567476
H23	1.7329222798	4.3734453965	13.3117019447
H24	2.3812198363	4.8800613081	11.7174095863
N26	1.4271294857	2.1069977197	12.8540644785
O27	1.4127589688	0.9935099715	12.4899730736
O28	1.5879032657	3.0072638529	11.7643056846

INT4: E=-552.40088541440

N1	0.5845331563	1.2022462126	1.1317382724
C2	-0.1126112504	2.3854206128	1.4783812114
H4	-0.7898281438	2.6847643515	0.6762965906
H5	0.5924218143	3.1874291032	1.6986580675
C6	1.6306034880	0.8183581595	2.0780949343
H7	1.2280921382	0.4664344301	3.0389380005
H8	2.2824292003	1.6744845998	2.2683105688
H9	2.2455518422	0.0242942969	1.6514855273
C10	-0.2494716067	0.0880078942	0.6692694930
H11	-1.2035628637	0.4990682099	0.3336784134
H12	-0.4771348129	-0.6171094540	1.4815912144
N13	-0.3446050001	-1.8597718941	-0.8797829561
C14	0.4734803351	-2.8109864966	-1.6206170098
H15	0.8486121291	-2.4089911924	-2.5810131876
H16	1.3341293890	-3.1110439601	-1.0178803643

H17	-0.1125491855	-3.7075712012	-1.8385509985
C18	-1.5524230702	-1.5244207186	-1.6242100690
H19	-1.3372311989	-1.0042187407	-2.5772839826
H20	-2.1055669282	-2.4381271788	-1.8540931694
H21	-2.2092839404	-0.8864678274	-1.0306198002
C22	0.4189709731	-0.6808155689	-0.4787497905
H23	1.4021637767	-1.0231839907	-0.1450914094
H24	0.5946991129	0.0137488722	-1.3212915083
N24	-2.3044516259	2.1671688030	2.3714139795
O25	-0.9250475959	2.2745018728	2.7001379874
O26	-2.9640790629	2.0322722572	3.3301108041

INT5: E=-552.40147970996

N1	0.5330163997	1.4139977515	1.0384836611
C2	-0.0370906040	2.6973097753	1.1836827866
H4	-0.6155357964	2.9842919656	0.3075476302
H5	0.7142667461	3.4412846788	1.4440368475
C6	1.4505532760	1.0113951998	2.1035781223
H7	0.9358574789	0.7721269829	3.0451829488
H8	2.1606730543	1.8174006769	2.2986047430
H9	2.0158009242	0.1341836200	1.7861699184
C10	-0.3566131314	0.3509586201	0.5506672854
H11	-1.2258575238	0.8239202230	0.0930315108
H12	-0.7377141782	-0.2650749095	1.3766938100
N13	-0.4715628218	-1.6887470668	-0.8680290582
C14	0.3240894025	-2.7576770875	-1.4581535435
H15	0.8281379820	-2.4592392681	-2.3969122939
H16	1.0889501229	-3.0870197418	-0.7506626315
H17	-0.3184497869	-3.6135305985	-1.6798213154
C18	-1.5655956594	-1.3048108855	-1.7523488536
H19	-1.2117644317	-0.8690325694	-2.7062898060
H20	-2.1716086661	-2.1833856961	-1.9851048023
H21	-2.2193108031	-0.5776976826	-1.2678181426
C22	0.3546232747	-0.5553005853	-0.4634513755
H23	1.2608156625	-0.9565345240	-0.0019705194
H24	0.6817561989	0.0569295455	-1.3248720262
N24	-1.0652733832	2.7681783902	2.3632975356
O25	-0.6214145335	3.0265448390	3.4727857598
O26	-2.2234453803	2.4662414623	2.1112687687

INT6: E=-552.40487843493

N1	3.2035476167	7.6918425416	12.3839854490
C2	3.2198332633	9.1458039181	12.5328587294
H3	2.9157618018	9.4834655531	13.5351327669
H4	2.5442106024	9.5980761280	11.8047512379
H5	4.2309183493	9.5106529798	12.3373698517
C6	4.1735435350	7.0214355188	13.2492354082
H7	3.9401142908	7.1249325507	14.3190590177
H8	5.1584238248	7.4563587081	13.0653424842
H9	4.2293155774	5.9592763994	13.0128837007
C10	1.9089400401	7.1126509198	12.2692268348

H11	1.2968144077	7.7345197783	11.6188862499
N13	0.5019666180	5.2546330541	11.5164110789
C14	0.2165461215	3.8651397572	11.8519928637
H15	0.8071599259	3.1415580058	11.2602042634
H16	0.4170383596	3.6950286999	12.9115197622
H17	-0.8417620778	3.6596096512	11.6737509337
C18	0.1278787239	5.5700730688	10.1443631889
H19	0.6953131775	4.9813810467	9.3995662400
H20	-0.9364488630	5.3725377795	9.9977741185
H21	0.2965465414	6.6288480056	9.9341822678
C22	1.8690280931	5.6505581973	11.8363371236
H23	2.2257493531	5.0328656714	12.6595138357
H24	2.5648189331	5.5259606132	10.9901482103
N24	1.1315695551	7.2267079805	13.6405401249
O25	1.3662316055	6.3915383599	14.5040071662
O26	0.4401003194	8.2217932166	13.7935917420

INT7: E=-346.62141980291

N1	3.0705417415	7.2685045832	13.2492087671
C2	3.1207997182	8.7222986862	13.3217313746
H3	2.2601158198	9.1599648031	13.8567874965
H4	3.1366834681	9.1390636455	12.3117599200
H5	4.0372623277	9.0343651857	13.8295714691
C6	3.1919219834	6.6103466401	14.5327521938
H7	2.2809140994	6.6943978132	15.1533874877
H8	4.0237795546	7.0508496035	15.0863753601
H9	3.4056131459	5.5481955908	14.3874826713
C10	2.1151804509	6.7564648618	12.3543537702
H11	2.0881696965	7.2939683538	11.4134617165
N13	0.3473954144	5.1899295705	11.6698878732
C14	0.3024399321	3.7358369417	11.5919169080
H15	1.1642074173	3.3039134493	11.0541560182
H16	0.2894151594	3.3155035521	12.6004619037
H17	-0.6135666828	3.4226197071	11.0840280483
C18	0.2234996150	5.8511271155	10.3877354875
H19	1.1331028990	5.7681416607	9.7652061757
H20	-0.6098143566	5.4119513005	9.8353786166
H21	0.0102959353	6.9129338724	10.5363974663
C22	1.3038669981	5.7014347794	12.5643270921
H23	1.3300806341	5.1643755399	13.5056238270

INT8: E=-552.39767775776

N1	3.4167073526	7.5240558856	12.5279405039
C2	3.5747481528	8.9756898955	12.4506589870
H3	3.0927204899	9.5073941560	13.2853472273
H4	3.1494513477	9.3451480227	11.5148159170
H5	4.6392960840	9.2223673732	12.4560883122
C6	4.0770062417	6.9811613721	13.7129699912
H7	3.6620535489	7.3741747021	14.6542660685
H8	5.1369026551	7.2441276837	13.6748319343
H9	4.0072800906	5.8946685084	13.7395606195

C10	2.0762108984	7.0806455002	12.2701265339
H11	1.7053420526	7.6821140585	11.4391036121
N13	0.6638197563	5.0524550936	11.8392931825
C14	0.6713856835	3.6074489918	11.6667181999
H15	1.0940567729	3.2849440346	10.6965141143
H16	1.2577129763	3.1434797221	12.4638337110
H17	-0.3497356506	3.2248991634	11.7342857557
C18	-0.2103698755	5.7180435656	10.8848034940
H19	0.1728907105	5.6844620013	9.8472940804
H20	-1.1908163575	5.2374058431	10.8987130370
H21	-0.3548083426	6.7617118980	11.1710353082
C22	2.0131054648	5.5932753854	11.8748714709
H23	2.5857981365	4.9933110295	12.5815905059
H24	2.5258954612	5.5215814675	10.8977776431
N27	1.0315482152	6.4101748461	14.3364929636
O29	1.1168065479	7.4252319879	13.3220510953
O30	0.2342454044	6.7032539856	15.1419519007

INT9:

ON-N (CH<sub>3</sub>)C<sub>2</sub>H<sub>5</sub>N(CH<sub>3</sub>)<sub>2</sub> E=-437.86718821538

N1	0.4941550516	1.2906091974	0.1216747127
C6	1.3884529648	1.2665129929	1.2730802124
H7	1.1608286082	0.3860092657	1.8718652189
H8	1.2432390725	2.1729515384	1.8638373144
H9	2.4353273058	1.2431971678	0.9573529297
C10	-0.3508489466	0.1655260456	-0.2504170174
H11	-1.0726545852	0.5634694804	-0.9635257313
H12	-0.8964269492	-0.1932572064	0.6271448534
N13	-0.3992155234	-2.1502588183	-1.1422636520
C14	0.3756010795	-3.3796442536	-1.2627517484
H15	1.0816912803	-3.3677350308	-2.1138055892
H16	0.9469130012	-3.5515957192	-0.3473831350
H17	-0.3013345319	-4.2264658879	-1.3998363059
C18	-1.2494340879	-1.9532792421	-2.3120279984
H19	-0.6692511715	-1.8215342682	-3.2442190135
H20	-1.9032311047	-2.8193767476	-2.4370560530
H21	-1.8874883501	-1.0773815721	-2.1840449286
C22	0.4480706961	-0.9966430751	-0.8610104752
H23	1.2121135774	-1.3091104277	-0.1430211840
H24	0.9811834613	-0.6319212028	-1.7587530339
N24	0.4523104710	2.3576620203	-0.6775909058
O26	1.2097793021	3.2637326509	-0.3635032961

CH<sub>2</sub>O E=-114.53628713669

C2	0.2339696607	4.9062005526	2.3758304592
H3	-0.0892952651	5.9248878858	2.6746860964
H4	0.5901530360	4.8058162158	1.3292334509
O25	0.2005616823	3.9758141286	3.1330445273

INT10:

CH<sub>3</sub>NCHCH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> E=-307.30135601509

N1	0.2704203172	1.6331765767	0.8542143493
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C6	1.7234468164	1.6065702793	0.9028055669
H7	2.0340705393	1.6592258591	1.9514637067
H8	2.1015435568	2.5120316772	0.4204030095
H9	2.2068124474	0.7344677937	0.4457399059
C10	-0.4037572289	0.6243417514	0.4912422039
H11	-1.4930657145	0.7316215883	0.4994463894
N13	-0.9009135678	-1.3216556733	-0.9099284822
C14	-0.7497630783	-2.7629079343	-1.0526470372
H15	0.2395313671	-3.0608370660	-1.4489448297
H16	-0.8899052540	-3.2495268338	-0.0842785744
H17	-1.5131602678	-3.1452187403	-1.7348942298
C18	-0.8137848579	-0.6462915328	-2.1994088457
H19	0.1643884093	-0.7950473303	-2.6952873832
H20	-1.5942557932	-1.0220295013	-2.8651781093
H21	-0.9677487327	0.4275560209	-2.0724826480
C22	0.0381145522	-0.7631242236	0.0586117851
H23	0.0238925300	-1.4032705168	0.9496532404
H24	1.0755436160	-0.7694056001	-0.3179933288
HNO E=-130.50890629664			
H12	0.4809144174	1.2740573292	0.0000000000
N24	-0.2882883286	0.5363685279	0.0000000000
O26	0.2220859127	-0.5498519540	0.0000000000

INT11: E=-551.74951625324

N1	2.7126844829	7.1454457204	13.3445341158
C2	2.6812894315	8.5953881929	13.4665579785
H3	1.6635639806	8.9918865715	13.3485347669
H4	3.3144412922	9.0405879366	12.6979844772
H5	3.0615833480	8.8973961558	14.4457011039
C6	2.1428180973	6.3854850314	14.4476682756
H7	1.0609928096	6.2502498069	14.3387448687
H8	2.3446968603	6.9150124128	15.3805531831
H9	2.6155550806	5.4031966189	14.5091228114
C10	2.9328823966	6.5831114950	12.1146903825
H11	3.3098374562	7.2511601771	11.3507762953
N13	2.9748245982	4.6600519909	10.6078052274
C14	2.2995481362	3.4379447918	10.1824038820
H15	2.2604881979	2.6737276898	10.9795490943
H16	1.2847290888	3.6610248461	9.8550720239
H17	2.8340450494	3.0139916721	9.3302486639
C18	4.3911480431	4.4230672447	10.8792865523
H19	4.5594806745	3.7029154659	11.6999418420
H20	4.8555354086	4.0200551634	9.9762252359
H21	4.8924210928	5.3542646984	11.1381551577
C22	2.2725027432	5.3531075545	11.6469313006
H24	1.9170839326	4.7154899151	12.4677564743
N23	0.8540473988	5.8504031304	11.0552388733
O24	0.7634982484	6.1411381785	9.8759800409
O25	-0.0147846561	6.0298874588	11.9056637622

INT12: E=-551.74792698566

N1	2.9096029995	7.2701803565	13.2496233935
C2	3.3537501207	8.6574834103	13.1569653867
H3	2.6384874134	9.3662969596	13.6004425632
H4	3.5062384456	8.9293580416	12.1102890927
H5	4.3097031084	8.7626704211	13.6756816170
C6	2.8408105168	6.8095741990	14.6339589129
H7	2.1651122916	7.4221806430	15.2495486747
H8	3.8406773802	6.8557016621	15.0733107337
H9	2.4926136452	5.7796948894	14.6843070155
C10	1.8315828183	6.9406536752	12.3893842858
H11	1.9744433429	7.4721209905	11.4461367426
N13	0.6188957606	5.0009170523	11.3894104544
C14	0.6030430205	3.5650543252	11.1620764746
H15	1.3227196012	3.2553960912	10.3884078694
H16	0.8494373538	3.0446630407	12.0891925472
H17	-0.3962999891	3.2534365434	10.8500888805
C18	0.0922562181	5.8028401019	10.2946207313
H19	0.7916716901	5.8616474795	9.4452657731
H20	-0.8372324532	5.3528468741	9.9404614685
H21	-0.1314611484	6.8105135220	10.6440595100
C22	1.6348588552	5.4943673112	12.1859132760
H23	2.0587452512	4.7918623193	12.8868871521
N27	-0.1765866166	6.9989249682	13.8106328538
O29	0.5044689170	7.6720978837	12.7973435537
O30	-1.1714633826	7.5646834373	14.1061962967

INT13:

(CH<sub>3</sub>)<sub>2</sub>NCH<sub>2</sub>CHO E=-287.86820779136

C10	-0.0782531059	7.1072545295	11.4609305656
H11	-0.2098255938	8.1303454579	11.0372685289
N13	1.1604321264	4.9433693157	11.1703685377
C14	2.3328674539	4.3513977552	10.5409819982
H15	2.2021085861	4.1667765111	9.4575937932
H16	3.1991812260	5.0048143460	10.6731929413
H17	2.5580896757	3.3954946260	11.0195757916
C18	0.0062410434	4.0519763105	11.1107372798
H19	-0.3290359257	3.8597022485	10.0734289157
H20	0.2687890275	3.0935386495	11.5640844460
H21	-0.8188901884	4.4784424090	11.6783174662
C22	0.8812464641	6.2607034570	10.6496259127
H23	1.8133747808	6.8389071267	10.5966822119
H24	0.4862424501	6.2584952541	9.6074045782
O29	-0.6675324178	6.7701697865	12.4532354356

(CH<sub>3</sub>)<sub>2</sub>N-NO E=-264.54768185445

N1	2.0860631441	7.2594379264	14.1309033614
C2	2.0682663898	5.9210042486	14.6839812191
H3	2.3918625845	5.9267753311	15.7300153221
H4	2.7547031500	5.3131480774	14.0958085024
H5	1.0630924158	5.4900285679	14.6306142681
C6	1.2671936805	8.3155097030	14.7039996161
H7	1.5408592323	8.4837523569	15.7499054669

H8	0.2080351531	8.0460747814	14.6517946725
H9	1.4479594364	9.2188463639	14.1245574697
N27	2.8934798238	7.4509674338	13.0770383100
O30	2.9116911691	8.5751390000	12.6090893566

INT14:

CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> E=-173.86876805004

N13	0.2799402036	4.7569081662	10.4300043704
C14	0.0182760274	4.5809051598	11.8480242582
H15	-0.6562160193	3.7341283111	11.9980291751
H16	0.9546155513	4.3691466728	12.3680812113
H17	-0.4358339759	5.4747147087	12.3058193473
C18	-0.9092232042	4.8555128359	9.6008931476
H19	-1.5674051384	4.0049019544	9.7947724477
H20	-1.4739413557	5.7837163132	9.7855997893
H21	-0.6220478421	4.8340653853	8.5478133880
C22	1.3628967919	5.5481200416	10.0794345965
H23	2.2259818748	5.5040628137	10.7316407188
H24	1.5201565500	5.7117074807	9.0208208167

CHON(CH<sub>3</sub>)<sub>2</sub> E= -248.58358499238

N1	3.3941148267	8.0766248522	13.7749071732
C2	3.1802856821	9.4746893352	13.4593188897
H3	2.6676744925	9.9904685459	14.2792598005
H4	2.5636706309	9.5564144958	12.5625859841
H5	4.1308059631	9.9876961874	13.2730816879
C6	4.1973174965	7.7527654644	14.9425070919
H7	3.7445465586	8.1643275110	15.8511453883
H8	5.2094399463	8.1601732547	14.8429519454
H9	4.2500725018	6.6686324309	15.0231054468
C10	2.8742476863	7.0778444200	13.0046991645
H11	2.2910506933	7.4787911164	12.1535202442
O29	3.0125738165	5.8877716463	13.1987215877

NO E= -129.92669818535

N1	0.0000000000	0.0000000000	0.6122998678
O2	0.0000000000	0.0000000000	-0.5360503988

INT15

ON-CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> E= -303.83914800981

N13	0.2936241997	4.6508717656	11.5313740743
C14	0.0910103514	3.2764609479	11.0867879610
H15	0.1382002692	3.1749721597	9.9862602707
H16	0.8541523430	2.6350137234	11.5281879663
H17	-0.8865716657	2.9247750947	11.4232652805
C18	-0.7365804519	5.5552969588	11.0388959463
H19	-0.7591795121	5.6335320854	9.9362991320
H20	-1.7157463592	5.2024324225	11.3709022881
H21	-0.5818656327	6.5558393219	11.4498354071
C22	1.6230891752	5.1267678110	11.2576353023
H23	1.9846582222	4.9218089440	10.2279621494
H24	1.7066711555	6.1994918486	11.4458294902

N27	2.6031758038	4.4155543500	12.1560547764
O30	3.6307984607	5.0202513589	12.2951549186

INT16 E= -551.75375601345

N1	2.9325110931	7.1082834875	13.3582391264
C2	3.5152640147	8.4288612116	13.1280055678
H3	2.8586928725	9.2499848453	13.4569771938
H4	3.7252559640	8.5618512546	12.0632631870
H5	4.4622911876	8.5068791319	13.6683262709
C6	2.7347279624	6.8753941560	14.7905781402
H7	2.0354723972	7.5914109033	15.2437109254
H8	3.7004501918	6.9526607019	15.2966902716
H9	2.3421857752	5.8729461886	14.9679709294
C10	1.7171947657	6.9118104861	12.5552354881
H11	1.9770403742	7.3001924977	11.5552781778
N13	0.8355386410	4.9041950113	11.3532045470
C14	0.7575059010	3.4627632414	11.1413218904
H15	0.9789189499	3.2291320276	10.0961823313
H16	1.4837108435	2.9566365918	11.7760665575
H17	-0.2448941482	3.0923387546	11.3786955046
C18	0.0087538009	5.7325802529	10.4698403092
H19	0.5036722156	5.8697400568	9.5025663387
H20	-0.9488410721	5.2333908075	10.3075759409
H21	-0.1770463410	6.6932524849	10.9474796556
C22	1.4513716365	5.4123079213	12.4160964756
H23	2.0625271814	4.7110682901	12.9726005991
N27	-0.0746324458	5.9608103303	13.7848973197
O29	0.5484838381	7.4890454097	12.9954407353
O30	-1.1698537097	5.7249211055	13.4392840847

INT17: E= -551.75588187683

N1	2.9286473405	7.2053854949	13.3916323202
C2	3.4507803898	8.5628128234	13.2367981230
H3	2.8093890533	9.3275856170	13.7027236962
H4	3.5568530256	8.7994020632	12.1755692548
H5	4.4415082231	8.6224736909	13.6939491991
C6	2.8484641147	6.8241133229	14.8023026545
H7	2.1634402299	7.4636066523	15.3758448270
H8	3.8457283835	6.8930987373	15.2426957187
H9	2.5124202291	5.7916791168	14.9083047205
C10	1.7399144311	6.9746181908	12.6266151627
H11	1.8864992549	7.4275756172	11.6446994230
N13	0.9853762618	4.9675104092	11.2720371191
C14	0.7032972822	3.5320697225	11.2592732524
H15	0.7700471640	3.1624520016	10.2334084373
H16	1.4491287216	3.0058885146	11.8585110869
H17	-0.2955089311	3.2957781898	11.6506610031
C18	0.1175074794	5.7304203772	10.3747211965
H19	0.2021842383	5.3155936224	9.3680754486
H20	-0.9329262378	5.6969626463	10.6916754904
H21	0.4250037632	6.7746064409	10.3372918799



C22	1.2713258254	5.5111473399	12.5296485250
H23	1.8445210662	4.7978039578	13.1181884948
N27	0.0147449147	5.9888329963	13.3966235315
O29	0.4930548251	7.4491247692	13.1934785892
O30	-1.1483681122	5.7221812963	13.1558630794

INT18:

ON-CHN(CH<sub>3</sub>)<sub>2</sub> E= -303.23631843486

N13	0.7032141179	4.7189029669	11.0025732713
C14	0.6089933271	3.7107181989	9.9554177966
H15	0.2778757250	4.1808786981	9.0261485669
H16	1.5890077280	3.2637817378	9.7797278804
H17	-0.0992970229	2.9076750960	10.2092097851
C18	-0.5132549978	5.4881979367	11.2314696361
H19	-0.7762781783	6.0187786763	10.3120180594
H20	-1.3586786984	4.8440377899	11.5134714987
H21	-0.3515740086	6.2192381776	12.0186009303
C22	1.5953500575	4.4726640199	12.0287910286
H23	2.4698715125	3.8918642004	11.7649433327
N27	1.5054372479	4.8018230511	13.2718982387
O30	0.7062020386	5.5320583689	13.9003657689

INT19: E=-421.84366465814

N1	3.0360081180	7.3886402850	13.2340517122
C2	2.9120988172	8.8240792251	13.4868608408
H3	2.1113592667	9.0678815486	14.2026317260
H4	2.7021437352	9.3447004163	12.5494774478
H5	3.8564770302	9.2077093759	13.8805074970
C6	3.3912679893	6.6415751531	14.4364216842
H7	2.5760698820	6.5990346384	15.1742374506
H8	4.2534754579	7.1222537944	14.9031600565
H9	3.6860050395	5.6238969623	14.1763858190
C10	1.9649922765	6.8864656705	12.4560766726
H11	1.8417715239	7.4706023253	11.5486147310
N13	1.0220783465	4.7931256674	11.3339712898
C14	0.0950695410	3.7212415960	11.6974127439
H15	-0.0544144321	3.0621475489	10.8388004783
H16	0.5225958001	3.1260732745	12.5078258959
H17	-0.8876342449	4.0943742374	12.0258522657
C18	0.5417581921	5.5836709770	10.2049629679
H19	1.3410375186	6.2189925003	9.8205474363
H20	0.2507687457	4.9031681895	9.4021682847
H21	-0.3244349970	6.2133447926	10.4573634433
C22	1.4893823726	5.5048917153	12.4651529100
H23	1.8918073968	4.8233960643	13.2090352352
O29	0.6783505520	6.5605881946	13.0740643595

TMMDA: E= -308.52465252161

C1	4.1252713070	-3.4793264488	-3.3289412262
H2	4.1464989048	-3.5937186729	-2.2455091963
H3	5.1063410889	-3.7443315841	-3.7313665196

N4	3.1083321783	-4.3665165928	-3.8801655479
C5	1.8213144588	-4.2028835396	-3.2210761295
H7	1.5064425436	-3.1429352892	-3.1917229480
H8	1.0697300953	-4.7482158257	-3.8219031693
C9	3.0085543727	-4.2488943137	-5.3260666058
H10	2.2902535790	-4.9760594663	-5.7133046320
H11	2.6951364703	-3.2423315080	-5.6637191496
H12	3.9807408689	-4.4619000227	-5.7778170141
H21	3.9319280795	-2.4151182173	-3.5648211840
N16	1.8665630073	-4.6824572512	-1.8480854801
C18	0.7419163020	-4.2076609443	-1.0578441929
H19	0.7044331508	-3.1155055000	-1.0767014963
H20	-0.2344802129	-4.5919870723	-1.4103475710
H22	0.8669171754	-4.5230509968	-0.0188919652
C21	2.0109624922	-6.1313280944	-1.7768261141
H23	2.2033114762	-6.4345097036	-0.7445123673
H24	1.1076464917	-6.6645453153	-2.1304048962
H25	2.8546435719	-6.4348327148	-2.3960907938

INT20: E= -307.86775220843

C1	3.4297690720	-3.4764397448	-2.6633101667
H2	3.1289157046	-3.6363470986	-1.6270180557
H3	4.5163085233	-3.5780785924	-2.7287285849
N4	2.7941733920	-4.4672471389	-3.5240176401
C5	1.3411551366	-4.5147825948	-3.3614800129
H6	0.9485096119	-5.1159381887	-4.1888908153
C7	3.1823179930	-4.3003889962	-4.9173006416
H8	2.7444165822	-5.0953403212	-5.5265618934
H9	2.8737404400	-3.3279134085	-5.3461537780
H10	4.2694555538	-4.3710183675	-5.0041232784
H11	3.1640092890	-2.4387743611	-2.9420267092
N12	0.9032505073	-5.1134204089	-2.1184391197
C13	0.6730572215	-4.3105167894	-1.0095884987
H14	0.3607585430	-3.2932403688	-1.2104289100
H15	0.2822284397	-4.8082793748	-0.1307561346
C16	1.2963710297	-6.4960394408	-1.9016209042
H17	0.6948145403	-6.9175827009	-1.0932701146
H18	1.1104091767	-7.0760371258	-2.8094797267
H19	2.3579310440	-6.5971720353	-1.6442784154
H20	0.8794439220	-3.5141583400	-3.4256158291

INT21: E= -307.87102708064

C1	4.1627743985	-3.6067060754	-3.2940518280
H2	4.1278732056	-3.7702269876	-2.2188415787
H3	5.1044747472	-3.9958589619	-3.6902631806
N4	3.0402660073	-4.3002527711	-3.9168263932
C5	1.8230894812	-4.2949694932	-3.2324969899
H8	0.9603854640	-4.5839984392	-3.8429947577
C9	2.9649811620	-4.1207851075	-5.3556401754
H10	2.1807395464	-4.7582436261	-5.7684822478
H11	2.7512262438	-3.0770823528	-5.6396363869

H12	3.9150880759	-4.4101191591	-5.8116756445
H21	4.1253168416	-2.5212134718	-3.4830715159
N16	1.8560680807	-4.6811423881	-1.8730477210
C18	0.6866474484	-4.2295708699	-1.1338664348
H19	0.5669476583	-3.1525731669	-1.2603685553
H20	-0.2467600519	-4.7225779408	-1.4645661382
H22	0.8171484206	-4.4430518422	-0.0691944726
C21	2.1413347168	-6.1042951819	-1.6467630386
H23	2.3434137176	-6.2803535829	-0.5859745993
H24	1.3025845391	-6.7543268575	-1.9533787769
H25	3.0231157488	-6.3886759622	-2.2214927368

INT22: E= -513.08175159997

C1	3.5097851747	-3.4303435987	-2.7418928137
H2	3.2794761619	-3.5357158260	-1.6827066039
H3	4.5873156591	-3.5605282824	-2.8696308669
N4	2.8024639940	-4.4412783530	-3.5199564194
C5	1.3570931837	-4.4463051947	-3.3039520231
H6	0.9183749675	-4.9757178068	-4.1569572533
C7	3.1488632886	-4.3659229367	-4.9329275550
H8	2.6635593144	-5.1758235123	-5.4833649958
H9	2.8633120960	-3.4075737247	-5.4066863195
H10	4.2291618316	-4.4824415905	-5.0489749070
H11	3.2517144201	-2.4002846787	-3.0543098697
N12	0.9012741853	-5.1123866865	-2.0963200197
C13	0.5951209660	-4.3798835223	-0.9368652058
H14	0.1703348757	-3.4114381844	-1.1986343610
H15	-0.0895292052	-4.9373412830	-0.2924280417
C16	1.3257296141	-6.4951571401	-1.9274839921
H17	0.7348279562	-6.9620363764	-1.1357033095
H18	1.1479960709	-7.0441748166	-2.8563563241
H19	2.3890438188	-6.5932784730	-1.6800551629
H20	0.9318564042	-3.4271818196	-3.2964780315
N21	1.8001039444	-4.8898189115	1.0607053114
O22	2.7444574698	-4.6693849912	1.7199202250
O23	1.7518973722	-4.0417768442	-0.0753216285

INT23: E= -513.08299938240

C1	3.8095324527	-3.7806337831	-2.8924930650
H2	3.6716992945	-4.0546733539	-1.8473661688
H3	4.8459871868	-3.9830792201	-3.1720095643
N4	2.9146354137	-4.5730372424	-3.7298197812
C5	1.5281927343	-4.4949835104	-3.3030630980
H6	0.9235425320	-4.9568809520	-4.0976434250
C7	3.0722595379	-4.2694506862	-5.1448995807
H8	2.4376177360	-4.9277973505	-5.7439045183
H9	2.8203201195	-3.2226978472	-5.3988221620
H10	4.1097703328	-4.4419187621	-5.4399333107
H11	3.6314603018	-2.6936275032	-2.9986461333
N12	1.3030357080	-5.1658881408	-2.0348084947
C13	0.5510282434	-4.5715374420	-1.0324546646

H14	0.1045910247	-3.6226810365	-1.3257596473
H15	-0.2178867236	-5.2096673730	-0.5878879945
C16	1.5131537441	-6.6057309979	-1.9951101168
H17	1.7825256236	-6.9189995922	-0.9849936805
H18	0.6247512486	-7.1692498003	-2.3202767353
H19	2.3479364034	-6.8483777454	-2.6522892643
H20	1.1796911908	-3.4521938007	-3.1897581632
N21	1.3873531984	-4.1639661463	0.2651035259
O22	2.5768761566	-4.4142804719	0.3036207568
O23	0.7347661205	-3.6342807861	1.1479454662

INT24: E=-513.08309592078

C1	4.1883380421	-3.7277621661	-3.3164767031
H2	4.1610693709	-3.7943697189	-2.2309508914
H3	5.0798806276	-4.2376670972	-3.6903365319
N4	3.0016050272	-4.3789174611	-3.8740113258
C5	1.7843227426	-4.2161024010	-3.1671771661
H8	0.9609123136	-4.6464081216	-3.7544488643
C9	2.9056267628	-4.2817449336	-5.3263082794
H10	2.0613950993	-4.8734364715	-5.6845589332
H11	2.7762786702	-3.2478057368	-5.6804033403
H12	3.8197578049	-4.6849952947	-5.7679888481
H21	4.2497265403	-2.6653564708	-3.5923869358
N16	1.8506189575	-4.6585664600	-1.8041133127
C18	0.6184209174	-4.4048193313	-1.0574684273
H19	0.4109752968	-3.3367053037	-1.0112032411
H20	-0.2561497788	-4.9242376686	-1.4868258892
H22	0.7532081900	-4.7578049351	-0.0340166855
C21	2.2506706763	-6.0648252507	-1.6991936399
H23	2.3998179564	-6.3060848379	-0.6450877892
H24	1.4890330811	-6.7527439184	-2.1060390161
H25	3.1826761081	-6.2334790634	-2.2334695556
N21	1.3815400384	-2.6688291433	-3.1855657943
O22	1.9339685536	-1.9056835889	-2.4113530596
O23	0.6337222163	-2.3395425186	-4.0964893266

INT25: E= -513.08000660619

C1	4.3402365504	-3.9025465764	-3.2818714461
H2	4.3099878695	-3.9859391051	-2.1974112190
H3	5.1649317018	-4.5105838315	-3.6666169315
N4	3.0852438629	-4.3937992111	-3.8466569531
C5	1.8784379872	-4.1611315425	-3.1315638858
H8	1.0596593147	-4.6194890992	-3.7102961055
C9	2.9885905208	-4.2033314603	-5.2870990820
H10	2.0879194472	-4.6889756798	-5.6695411463
H11	2.9606050504	-3.1428959040	-5.5823589201
H12	3.8531205415	-4.6672649052	-5.7688521876
H21	4.5387145953	-2.8522140223	-3.5377753467
N16	1.9387710194	-4.6545039713	-1.7690849638
C18	0.7054892011	-4.4070930382	-1.0190433627
H19	0.4667835085	-3.3465696903	-1.0016577891

H20	-0.1606433780	-4.9482967111	-1.4404014267
H22	0.8490479740	-4.7448243750	0.0089646639
C21	2.2861587969	-6.0762717266	-1.7127463757
H23	2.3763984181	-6.3731504383	-0.6658528469
H24	1.5188728662	-6.7156008890	-2.1850173203
H25	3.2336713638	-6.2601331913	-2.2132096884
O21	1.4062483436	-2.7611917893	-3.1143627199
N22	2.3180235661	-1.8681546215	-2.4676583661
O23	1.8735194917	-0.7839614063	-2.4413056478

INT26:

ON-N (CH<sub>3</sub>)CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> E= -398.54826067720

C1	3.2674379571	-3.1649214292	-3.3774883229
H2	2.7508945476	-3.0180192447	-2.4281069974
H3	4.3402583742	-3.2093497209	-3.1772811433
N4	2.8344269695	-4.4160199600	-3.9926303177
C5	1.3893824474	-4.5099423988	-4.1109524019
H6	1.1585490666	-5.3582839547	-4.7634685010
C7	3.5091611832	-4.6647757917	-5.2604036778
H8	3.2129046368	-5.6390248623	-5.6572679886
H9	3.2954029713	-3.8988156207	-6.0277390904
H10	4.5891643239	-4.6826342916	-5.0982394882
H11	3.0684853109	-2.2859996984	-4.0160984446
N12	0.7557157372	-4.7152664602	-2.8197096750
C16	1.0014039678	-5.9124186130	-2.0263813743
H17	1.0916645252	-5.6330337004	-0.9763472353
H18	0.1698167152	-6.6184917450	-2.1167676673
H19	1.9275213208	-6.3611608207	-2.3793039449
H20	0.9151860690	-3.6094231440	-4.5304867653
N21	-0.0915301212	-3.7657702512	-2.4115363009
O22	-0.6457688736	-3.9900605170	-1.3478015287

INT27:

(CH<sub>3</sub>)NCHN(CH<sub>3</sub>)<sub>2</sub> E= -267.98910885213

N1	0.2797941813	1.7279400259	0.8788357057
C6	1.5285900770	1.2013067882	1.4031649088
H7	1.3658370349	0.5072680258	2.2398502834
H8	2.1104686417	2.0371300980	1.8050014296
H9	2.1465092980	0.6933353097	0.6494578819
C10	-0.4035423777	1.1481405705	-0.0262182923
H11	-1.2562487335	1.7143046880	-0.4128881461
N13	-0.2580604131	-0.0666468821	-0.6867127221
C14	0.2479980316	-1.2789689070	-0.0600684868
H15	0.8836497706	-1.8344245600	-0.7674554190
H16	0.8385289712	-1.0499354578	0.8293562659
H17	-0.5874606559	-1.9380232116	0.2415974121
C18	-1.1365927156	-0.3301912408	-1.8173506865
H19	-0.5902756160	-0.8664562423	-2.5993599076
H20	-2.0070613337	-0.9406856825	-1.5334687360
H21	-1.4915458527	0.6072766583	-2.2441799002

INT28: see INT13 and INT14

INT29: E=-909.16052821783

N1	0.7990100961	1.3187651591	0.5893653758
C2	0.3036346087	2.6756881002	0.8932017494
H3	-0.4333561529	2.6596872232	1.7048270473
H4	-0.1521283342	3.1041852482	-0.0013053348
H5	1.1465858697	3.3008509730	1.1854678975
C6	1.6026487900	0.7739109297	1.6041139441
H8	2.3331895327	1.4306221887	2.0528369427
H9	1.7470779922	-0.2955089353	1.6269254728
C10	-0.2573171162	0.4249599509	0.0691811788
H11	-0.9278252110	1.0429583652	-0.5294103803
H12	-0.8400762446	0.0043632830	0.8987598121
N13	-0.6884917615	-1.7156557142	-1.1611752649
C14	-0.0452207178	-2.8972612188	-1.7629971365
H15	0.4650910378	-2.6500420332	-2.7041292494
H16	0.6857236230	-3.3094307864	-1.0648396232
H17	-0.8061915589	-3.6540010149	-1.9536601019
C18	-1.7250793867	-1.1850204739	-2.0641224964
H19	-1.2919765763	-0.8161708129	-3.0047869970
H20	-2.4385536780	-1.9791279999	-2.2813442040
H21	-2.2682748720	-0.3716004041	-1.5823517169
C22	0.3221668404	-0.7034376536	-0.7945385266
H23	1.1058181861	-1.2206183444	-0.2374330321
H24	0.7910904213	-0.2823551575	-1.6960587530
N25	3.5218587116	2.6886646158	-1.1988287037
O26	3.5027753310	3.1299002604	-0.0651065039
O27	4.3002524552	2.9217558810	-2.0807418813
O28	2.5139915914	1.7979792320	-1.5378868436
H29	1.9565644240	1.6704419985	-0.7093384516
N30	-2.8117574506	-3.4705814204	0.8001036508
O31	-2.9999414093	-3.7604717276	-0.3730687467
O32	-3.3906764258	-3.8982905513	1.7632438489
O33	-1.8295679917	-2.5532886526	1.0637062163
H34	-1.4220770187	-2.2613520442	0.1475397916

INT30: E=-909.16655626954

N1	0.9362396102	1.4876217786	0.7898025705
C2	0.1915877469	2.7271369569	1.0682507268
H3	-0.1903585453	2.7435164883	2.0966865967
H4	-0.6484361515	2.8067925244	0.3771680336
H5	0.8532427633	3.5791218546	0.9129884915
C6	2.1465433174	1.3847007309	1.6318113924
H7	1.8828083567	1.3394620643	2.6962442691
H8	2.7770586502	2.2541461595	1.4466401898
H9	2.7115211897	0.4898516842	1.3727349449
C10	0.1205319805	0.3407911316	0.7225282221
H11	-0.9489942105	0.4978209392	0.6900405788
N13	-0.1871723148	-1.8123286619	-0.4441934958
C14	0.2056346948	-3.2309332595	-0.4460839956

H15	1.2212588493	-3.3729147226	-0.8417491057
H16	0.1657610550	-3.6229583980	0.5721644620
H17	-0.4996325004	-3.7909307266	-1.0598395093
C18	-0.2016097282	-1.2753643381	-1.8169179228
H19	0.7872403706	-1.3491273882	-2.2895322296
H20	-0.9296518703	-1.8341385175	-2.4046493040
H21	-0.4970025462	-0.2261457853	-1.7992788880
C22	0.6826614902	-1.0172194887	0.4563993679
H23	0.7777124776	-1.5984707294	1.3846393989
H24	1.6965760013	-0.9436360233	0.0304319757
N25	2.6677291594	2.8416333214	-1.9062953954
O26	2.8545046841	3.5086596936	-0.9031074854
O27	3.1127511743	3.0117080313	-3.0069733034
O28	1.8384074485	1.7428342171	-1.7780255178
H29	1.5447538958	1.7192400359	-0.8077036436
N30	-3.5109249103	-2.3455036364	-0.2512515561
O31	-3.0579851140	-2.9560192859	-1.2093561074
O32	-4.6599977585	-2.2839669477	0.1005321831
O33	-2.6216077610	-1.6490958640	0.5201292831
H34	-1.6702371303	-1.7655301977	0.0897559812

INT31: E=-869.83624706556

N1	0.0873721589	0.4532665222	1.3825992760
C2	-0.5975928560	-0.4386118175	2.3356796408
H3	-0.0005582680	-1.3320235830	2.5574454187
H4	-1.5620412987	-0.7497354027	1.9373458647
H5	-0.7753547474	0.1097656559	3.2620967673
C6	1.3366546461	0.9744977135	1.9744623648
H7	2.0500123780	0.1690000489	2.1953965169
H8	1.1004177122	1.4958698746	2.9031277143
H9	1.7944544372	1.6847451105	1.2854390449
N10	-0.7449707761	-0.7082300831	-0.6407176663
C11	-0.3533121567	-1.4903491635	-1.7429313511
H13	0.4665973321	-2.1780052212	-1.5908596431
H14	-1.1149303986	-1.7143881379	-2.4759053767
C15	-1.7620118275	0.3084634068	-0.9680160962
H16	-1.3360646428	1.1136149869	-1.5767977362
H17	-2.5665605913	-0.1725909879	-1.5249664031
H18	-2.1807669376	0.7327971904	-0.0577543195
C19	0.4197993437	-0.1988638345	0.1053629870
H20	1.0802379764	-1.0579817200	0.2779313733
H21	0.9497449812	0.5427058311	-0.5017070313
H26	-0.7421684584	1.8512089720	1.2568157871
N27	-1.2845565912	-3.8564324297	0.9819396415
O28	-2.1584176227	-2.8991793023	0.4832849955
O29	-1.8115762231	-4.8560241364	1.3792067539
O30	-0.0999174559	-3.5746622947	0.9642988188
H31	-1.5809635872	-2.1495566167	0.1616626761
N37	-0.7331873385	3.6076890801	0.4225364968
O38	0.1844261832	3.1846679203	-0.2665413867
O39	-1.2313715229	4.6999480025	0.3938854737

O40	-1.2698464642	2.7399430504	1.3416780085
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INT32: E=-869.84092992707

N1	0.1946492711	0.3774385329	1.0912116132
C2	-0.5701389006	-0.3221101335	2.1578778807
H3	-0.0153526796	-1.1861817736	2.5430475842
H4	-1.5281808637	-0.6637533424	1.7689567592
H5	-0.7593966750	0.3777249524	2.9740621576
C6	1.4772444064	0.8873707142	1.6147289392
H7	2.1376203972	0.0697085652	1.9336827492
H8	1.2826211857	1.5336987468	2.4721419883
H9	1.9707790421	1.4700742110	0.8376758269
N10	-0.6622121671	-0.8620007513	-0.8411947303
C11	-0.2105440407	-1.5878081608	-2.0454110133
H12	0.2936224324	-0.9171090027	-2.7507803824
H13	0.4716600201	-2.3850041076	-1.7502251660
H14	-1.0762718845	-2.0360358760	-2.5347954171
C15	-1.6925457869	0.1438579324	-1.1724582567
H16	-1.2799383720	0.9347884373	-1.8088741009
H17	-2.5091710440	-0.3546577978	-1.6961569227
H18	-2.0914539553	0.5943607081	-0.2660131711
C19	0.4309814323	-0.3955881243	-0.0796066236
H20	1.2999272834	-1.0495979902	-0.0845239101
H26	-0.5829856103	1.8597078443	0.8616605349
N27	-1.2358826168	-3.9080989701	0.7575908085
O28	-2.0818368437	-2.8995903209	0.3268621876
O29	-1.7893683173	-4.8669142217	1.2176851456
O30	-0.0402361105	-3.7135535088	0.6243016750
H31	-1.4829737518	-2.1678936592	-0.0400472663
N37	-0.5715793907	3.5812154925	-0.0308138356
O38	0.2971104562	3.1167266022	-0.7486720270
O39	-1.0506607975	4.6817615411	-0.0589622502
O40	-1.0841342692	2.7478167593	0.9436331125

TS1: E= -552.95666119560

N1	2.7560737663	7.5978168390	12.7732327111
C2	3.3639495674	8.9036330588	12.5475525897
H3	2.7077928349	9.7465898550	12.8345869125
H4	3.6256713084	9.0155218837	11.4931281168
H5	4.2846262837	8.9821883247	13.1309866118
C6	2.4987055672	7.3774156318	14.1908106265
H7	1.7889401414	8.1124882219	14.6151575489
H8	3.4350198537	7.4458965213	14.7495019456
H9	2.0894880644	6.3792940459	14.3593124989
C10	1.5726381863	7.3795949500	11.9446028127
H11	1.7175098568	7.9166089419	11.0049524657
H12	0.6559513459	7.7832745851	12.4120994716
N13	0.1056500644	5.5428050243	11.0419717830
C14	-0.1903621699	4.1170232553	11.0263108020
H15	0.4855584351	3.5914171490	10.3393726012
H16	-0.0710029276	3.7059143689	12.0307759701



H17	-1.2202318396	3.9609727964	10.7017844322
C18	-0.3660597428	6.2943811136	9.9718203126
H19	0.4039030063	6.0927125955	8.8051410708
H20	-1.3618851181	5.9939629935	9.6477065017
H21	-0.2673716112	7.3702028235	10.1019395964
C22	1.3927276752	5.8854677534	11.6498262989
H23	1.4654132065	5.3180190256	12.5800783296
H24	2.2066369088	5.5427441646	10.9964351217
N26	1.8922597583	5.1542684262	7.6401562101
O27	0.9715576712	6.0758404251	7.7242554617
O28	2.0689258840	4.4602297795	8.6142772359

TS2: E=-552.95687257360

N1	2.9677032345	7.3050269411	13.3909029817
C2	3.5678726276	8.6241729589	13.2462880761
H3	2.8711715955	9.4514873136	13.4795950825
H4	3.9321498018	8.7539467255	12.2251972919
H5	4.4245032481	8.7084815286	13.9194639423
C6	2.5854129942	7.0351774871	14.7696922109
H7	1.8251481037	7.7438020634	15.1501940381
H8	3.4641052286	7.0975902619	15.4159511696
H9	2.1778103500	6.0259133622	14.8615747598
C10	1.8765106809	7.0687606685	12.4524829057
H11	2.0649105625	7.6643443925	11.5548309287
H12	0.9035852097	7.4105293156	12.8592043208
N13	0.6081104037	5.1009735612	11.5456723672
C14	0.4958614013	3.6568013146	11.3913309930
H15	1.0323918961	3.3169397078	10.4961107272
H16	0.9145944809	3.1613568027	12.2683388148
H17	-0.5572447993	3.3803694546	11.3021748075
C18	-0.0609614076	5.8666050894	10.5021321001
H19	0.4626853789	5.7533607213	9.5430453269
H20	-1.0846172933	5.5038485717	10.3896577500
H21	-0.0982856994	6.9224632078	10.7680711801
C22	1.7993267674	5.5880876977	12.0835191291
H23	2.1800988837	4.9318863241	12.8666090903
H24	2.8452691292	5.4813613098	11.1500048661
N26	3.7053987781	5.0433134830	9.2643156516
O27	3.8537663858	5.5578806810	10.4523205635
O28	2.6253382233	4.5667005900	8.9982243193

TS3: E= -758.09110326314

N1	3.4390158809	6.6458023205	13.2166043874
C2	3.4811733091	6.6982068151	14.6750207729
H3	3.9450844064	5.7879926636	15.0588003785
H4	2.4698876682	6.7924473237	15.0667311097
H5	4.0665076850	7.5671030864	14.9940135296
C6	4.7319013185	6.6138625534	12.5362171637
H7	5.3789567986	5.8892069361	13.0287820061
H8	5.1973774377	7.6057574993	12.5763368212
H9	4.5947368577	6.3129539314	11.5002493774

C10	2.2863302154	6.7153957460	12.5521642914
H11	2.3640616775	6.9026377388	11.4876751749
H12	1.4144148648	7.1749904040	13.0514783248
N13	0.1490435886	5.0018104596	11.9440608009
C14	-0.0326594432	5.1411445911	10.4993046787
H15	-0.2994401304	6.1707529119	10.2463559165
H16	0.8941992495	4.8739404185	9.9933590495
H17	-0.8284953989	4.4700604802	10.1667178663
C18	-1.0564340814	5.0667014662	12.7690773833
H19	-1.4810803415	6.0728390943	12.7543361897
H20	-1.7921159369	4.3517042056	12.3904177675
H21	-0.8042371144	4.8099947887	13.7967524713
C22	1.3729493114	4.9543406161	12.4708924407
H23	1.4229099482	4.7157999389	13.5279191214
H24	2.1917904166	4.5359476648	11.8569021686
N26	4.2548243087	3.2342603701	12.4488809390
O27	3.6786200619	3.4709055097	11.3744962256
O28	3.8732403435	3.7936186250	13.4868633113
N29	-0.3302537280	8.6659894776	12.0352755626
O30	-0.2037006035	8.1794628688	13.1752588375
O31	0.5602329335	8.5065343328	11.1953858163

TS4: E= -552.35107422392

N1	0.5732160199	1.5872042915	0.6976687837
C2	-0.2081634910	3.1018411384	1.3253305262
H3	-0.4630465287	2.8042906486	2.3646321606
H4	-1.0928690049	3.0298047706	0.6591525620
C6	1.7409012391	1.2417281507	1.4864744177
H7	1.4640038643	0.5266005742	2.2658589619
H8	2.1133639416	2.1635153241	1.9380470591
H9	2.5397563947	0.8083170417	0.8744430998
C10	-0.2878887824	0.5023953267	0.2259157835
H11	-1.0575725725	0.9688848941	-0.3942466026
H12	-0.7974858908	0.0620553701	1.0907650475
N13	-0.5274310843	-1.6458199603	-0.9780489655
C14	0.1220989925	-2.9319679563	-1.2050639727
H15	0.8580941126	-2.9090931992	-2.0301322011
H16	0.6355783923	-3.2562231063	-0.2969250370
H17	-0.6326587568	-3.6833282246	-1.4495600594
C18	-1.3082418182	-1.2444468796	-2.1436879242
H19	-0.6834878719	-1.0928056402	-3.0437288123
H20	-2.0487281849	-2.0150715488	-2.3694221875
H21	-1.8503728627	-0.3178202223	-1.9481037834
C22	0.4198845685	-0.6199730244	-0.5499233026
H23	1.1517923055	-1.0957313213	0.1071446175
H24	0.9834899196	-0.1967638574	-1.4021731767
N24	1.0752627691	2.5361000975	-0.6824620470
O25	0.6678969289	3.9831269149	1.1222184396
O26	2.2100258232	2.4841118507	-0.8608800429

TS5: E= -552.32730776692

N1	0.0503252823	1.8592228209	0.8876811011
C2	-0.8694711687	2.7202552515	1.8401060728
H4	-1.7467076818	2.9471908400	1.2022644502
H5	-0.3093642752	3.6553244876	2.0163060497
C6	1.3847227193	1.6232067249	1.4485373191
H7	1.2993383484	1.2838008736	2.4815541669
H8	1.9303542803	2.5691243253	1.4308161708
H9	1.9354097870	0.8923035759	0.8590040980
C10	-0.6305313790	0.9116504347	0.2628975079
H11	-1.5455024021	1.2321867446	-0.2325631153
H12	-1.6386176725	0.4296319188	1.4541456930
N13	-1.0569417215	-1.1870499104	-0.8968659798
C14	-0.9564073575	-2.6317218782	-0.7143777994
H15	0.0141569189	-3.0453506521	-1.0433868379
H16	-1.1009491158	-2.8817999239	0.3382784438
H17	-1.7441098235	-3.1231507992	-1.2897481592
C18	-0.9682960171	-0.8127983613	-2.3034641685
H19	-0.0005660696	-1.0927679479	-2.7597350037
H20	-1.7660150251	-1.3026127264	-2.8657365101
H21	-1.0942471011	0.2666366486	-2.4186848161
C22	-0.1072003357	-0.4546373644	-0.0715833652
H23	0.0204383858	-0.9839429496	0.8879911106
H24	0.8998225408	-0.4000358729	-0.5263837517
N24	-1.9163775230	0.1673814038	2.5204936792
O25	-1.0734818586	1.9959203276	2.9243666986
O26	-1.1871515975	-0.6778920234	2.9417850461

TS6: E= -757.51849343698

N1	2.8955659328	7.5620091225	12.9469501489
C2	3.1043456625	8.9971213102	13.0998165345
H3	2.4978046766	9.4319972208	13.9084422160
H4	2.8566379485	9.5091757109	12.1669558829
H5	4.1567707554	9.1867448648	13.3203834393
C6	3.3762990469	6.7708997393	14.0803587065
H7	2.7703700524	6.9062459265	14.9834472408
H8	4.4018984849	7.0796932468	14.2923318159
H9	3.4140365329	5.7136323541	13.8220447505
C10	1.7220541172	7.2082720786	12.2652214386
H11	1.6343465457	7.7962557667	11.3529822843
N13	0.4929608306	5.3331534778	11.1753258595
C14	0.2150999961	3.9036014723	11.1351182774
H15	0.9067205767	3.3975891140	10.4478387655
H16	0.3250938487	3.4764066181	12.1321983924
H17	-0.8078953891	3.7402691048	10.7918493603
C18	0.2421583881	6.0351367062	9.9210709011
H19	1.0803778458	5.8814381463	9.2284709656
H20	-0.6652499736	5.6303599198	9.4727514751
H21	0.0818032729	7.0957499796	10.1031202018
C22	1.5376518599	5.7287656674	12.0132075126
H23	1.5213545878	5.1500487433	12.9366116129
H24	2.7434477856	5.3215803868	11.4887237249

N26	4.0313938250	4.4388645572	10.0223542154
O27	3.9035585490	4.9207105589	11.2192408616
O28	3.0524655723	4.4297830300	9.3118246203
N27	0.3770369625	7.7005745549	13.0473806964
O29	0.3491360317	7.5507861060	14.2579647968
O30	-0.5083689162	8.1972544694	12.3697421825

TS7: E=-551.74877572763

N1	2.6573293113	7.0935710798	13.4117824030
C2	2.7498698926	8.5406745635	13.5343784868
H3	1.8009323074	9.0328069382	13.2807354487
H4	3.5228761698	8.9165314007	12.8622468436
H5	3.0213889528	8.8119218880	14.5574465666
C6	1.8734894714	6.4061421446	14.4275565844
H7	0.8069320093	6.3860857764	14.1776566642
H8	2.0109529708	6.9175042633	15.3819217161
H9	2.2280375365	5.3794450035	14.5416919607
C10	2.9367536825	6.5156059341	12.1992106866
H11	3.4642926853	7.1506420859	11.5003931518
N13	2.9072555369	4.5864633825	10.6921252707
C14	2.2876682345	3.3036095732	10.4054685188
H15	2.4930576723	2.5465420729	11.1820751916
H16	1.2078014511	3.4244440439	10.3111998718
H17	2.6589812976	2.9241822300	9.4512100609
C18	4.3588012219	4.5822406728	10.5818681267
H19	4.8443027979	3.9429831789	11.3379112704
H20	4.6340316983	4.2076572096	9.5926235903
H21	4.7631058181	5.5868795386	10.6817196446
C22	2.2670376056	5.3391022041	11.6898525319
H24	1.7468648610	4.7563760325	12.4543605989
N23	0.7842822433	5.9569030856	10.9342097891
O24	0.7540666958	6.0990302212	9.7289829097
O25	-0.0753402228	6.3326080450	11.7241666142

TS8: E= -551.74587462438

N1	2.8713331508	7.2565457540	13.4903938706
C2	3.1232192824	8.6940269293	13.5254606410
H3	2.3347475145	9.2465780630	14.0547649364
H4	3.1890734785	9.0826190768	12.5073859444
H5	4.0773625131	8.8796870077	14.0240608800
C6	2.9289313357	6.6421463297	14.8145487414
H7	2.1343608789	7.0040394796	15.4798302702
H8	3.8968769418	6.8767453279	15.2638307295
H9	2.8462390710	5.5590284408	14.7487937904
C10	1.8863447167	6.8531051923	12.5858557557
H11	1.9583926433	7.4453482964	11.6754055228
N13	0.9692966073	4.9103120151	11.3304356422
C14	0.5848417630	3.5106780592	11.4317498984
H15	0.3808071311	3.1117112177	10.4355629053
H16	1.4022299199	2.9351585502	11.8689405111
H17	-0.3116264910	3.3717134934	12.0539679156

C18	0.0707750167	5.7378365202	10.5369218711
H19	-0.1671957013	5.2094435737	9.6114533884
H20	-0.8612589210	5.9676377266	11.0697163963
H21	0.5446681950	6.6822565005	10.2744052901
C22	1.7149601622	5.4336929163	12.3652422975
H23	2.1407126807	4.7128396736	13.0432183744
N27	-0.1755337976	6.8942712853	14.0399696035
O29	0.3834862671	7.5457376002	12.9886525620
O30	-1.2265759643	7.3645810217	14.3555469204

TS9: E=-757.51343893607

N1	2.8574232831	7.3648812709	13.1849811953
C2	3.2839695687	8.7605521091	13.1170926265
H3	2.5826134378	9.4499212965	13.6110169798
H4	3.3940920806	9.0625166231	12.0737321836
H5	4.2594217469	8.8587553187	13.5984885396
C6	2.8412258969	6.8623341496	14.5554504366
H7	2.1451899281	7.4149356028	15.2051658717
H8	3.8455503025	6.9565453749	14.9746402267
H9	2.5659026783	5.8092517859	14.5871433528
C10	1.7543844248	7.0476079009	12.3447950116
H11	1.8823358783	7.6093607103	11.4187335458
N13	0.5469753082	5.1006614807	11.3450536179
C14	0.4095443577	3.6577874158	11.2086835538
H15	1.0342449248	3.2875293887	10.3851757327
H16	0.7119011627	3.1701144521	12.1361606690
H17	-0.6336356557	3.4090557334	11.0042920569
C18	0.0093921558	5.8748233098	10.2336774702
H19	0.6854482304	5.8238091995	9.3695722246
H20	-0.9568864935	5.4572302741	9.9476019665
H21	-0.1408953280	6.9107200571	10.5345598296
C22	1.6692730694	5.5603061547	12.0300229270
H23	1.9074365100	4.9102473368	12.8690244693
H24	2.8081648770	5.3887763980	11.2543445378
N26	3.8785224892	4.8280111819	9.4938451974
O27	3.9196413304	5.3240690611	10.6934994343
O28	2.7976974869	4.5000470145	9.0588874212
N27	-0.1709745974	6.7997051317	13.7981790555
O29	0.4499405177	7.6132890507	12.8080024456
O30	-1.1809666670	7.2781498567	14.1542621287

TS10: E= -552.36257716219

N1	1.9183621969	7.3267974889	13.3566102682
C2	3.3439991931	7.4359930326	13.6281803285
H3	3.5388176554	7.7816108857	14.6509345019
H4	3.7913589028	8.1417557483	12.9250742003
H5	3.8261134527	6.4614218057	13.4979775965
C6	1.1587626640	6.5332795196	14.3032529255
H7	1.1317606052	7.0204750058	15.2869818048
H8	1.6089353532	5.5439372981	14.4042311662
H9	0.1439452678	6.4258816532	13.9233193376

C10	1.3087613829	7.2755762219	11.6375283051
H11	2.1208899446	7.9441203762	11.2718795295
N13	0.6621424839	4.8278236692	11.5960146937
C14	1.2048399274	3.4967481509	11.3575089035
H15	1.3131272543	3.2582247592	10.2821230154
H16	2.1872258572	3.3971414401	11.8274968750
H17	0.5421399301	2.7482680619	11.7997166752
C18	-0.6933262691	4.9424377081	11.0559375636
H19	-0.7221740601	4.7504806580	9.9663229968
H20	-1.3432796249	4.2133808588	11.5473837419
H21	-1.0702839057	5.9457631919	11.2433820954
C22	1.5482296463	5.8653739983	11.0872669665
H23	2.5827773896	5.5882624423	11.3170140117
H24	1.4911113319	5.9561583100	9.9822670568
N27	1.2768917959	8.9736515217	13.3870200697
O29	0.1482787985	7.7577005268	11.7714930307
O30	0.6261161557	9.1719229082	14.3126736672

TS11: E= -552.35095745045

N1	3.1234526765	7.6521417885	13.0677767728
C2	4.2816146209	7.9130206787	12.2461840963
H3	5.0169731498	8.4953435190	12.8104834950
H4	3.9921411930	8.4975613991	11.3691205615
H5	4.7880065986	6.9964869733	11.8941938647
C6	3.3777337412	6.9542953391	14.3094562974
H7	4.1088624364	7.5158697527	14.8997476825
H8	3.7786963349	5.9362942139	14.1585941890
H9	2.4505566259	6.8819464555	14.8709368090
C10	1.8628301165	7.5021430853	12.4177138463
H11	1.7953432336	8.2706105180	11.6256210167
N13	1.2828482754	4.9035813700	11.6039502583
C14	2.0064851072	3.7014500725	11.9734988816
H15	2.2193026181	3.0666953370	11.1001698067
H16	2.9519309811	3.9719110038	12.4454319677
H17	1.4244511081	3.1187063173	12.6904303740
C18	-0.1131104628	4.7628235241	11.2350390900
H19	-0.2267650434	4.3987103647	10.2029543660
H20	-0.6113100819	4.0636978751	11.9083576185
H21	-0.6020936522	5.7320422738	11.3361363144
C22	1.9649681485	6.0235500223	11.1637512509
H23	3.0298272596	5.8541874517	11.0233015971
H24	1.4956830996	6.5073313528	10.3085321686
N27	0.5710084949	5.4713310837	14.0670585680
O29	0.8026719921	7.3012325844	13.1074985074
O30	-0.5601983367	5.3552623593	14.2489810307

TS12: E= -552.32397353143

N1	3.0428833489	7.6864426083	12.7346373200
C2	3.4205696551	8.5478790860	11.6307678531
H3	3.2678074111	9.6134723394	11.8698885604
H4	2.8322440868	8.3186098234	10.7411745033

H5	4.4760374327	8.4074138011	11.3789057050
C6	3.7794605180	7.9374108912	13.9655071062
H7	3.7111308230	8.9953941709	14.2668455828
H8	4.8359428476	7.6879647723	13.8271543131
H9	3.3698272259	7.3292651039	14.7661012771
C10	1.7006737600	7.2471407926	12.8005781181
H11	1.0150692345	7.7970312548	12.1444664891
N13	0.4253769852	5.2105457401	11.0572451156
C14	0.0997073873	3.8297686534	11.3516771710
H15	0.5910985828	3.1201375960	10.6633871176
H16	0.4094556124	3.5902581435	12.3690216374
H17	-0.9806474158	3.6784760119	11.2814990784
C18	-0.1851145764	5.7485903164	9.8551560422
H19	0.2115120427	5.2962668004	8.9289049042
H20	-1.2651879783	5.5795268576	9.8779413414
H21	-0.0186676134	6.8266427836	9.8031666071
C22	1.6890924422	5.6843222499	11.4269572509
H23	2.4578626447	4.9360764850	11.6207661773
H24	2.0740472696	6.3988323302	10.7052891210
N27	1.6197319815	5.1448491703	13.7930459725
O29	1.2222688076	6.9211167724	13.9697486045
O30	2.6596377390	4.8884097133	14.2019077505

TS13: E= -551.71801748059

N1	2.7901357753	7.2632260046	13.0081788544
C2	3.3976864079	6.2818662479	13.9106128456
H3	4.4180900744	6.5942408919	14.1309005810
H4	3.4302443105	5.3000889266	13.4389988571
H5	2.8224554906	6.2187102818	14.8377871934
C6	3.1882893701	8.6537011214	13.2273363163
H7	4.2764512949	8.7325678180	13.2082624424
H8	2.8136021889	9.0074038364	14.1935386965
H9	2.7725824761	9.2803635152	12.4392785684
C10	1.6275621646	7.0308103082	12.4142440356
H11	1.1897388233	7.8468634996	11.8570470497
N13	0.2831814960	5.5349192395	11.0361256731
C14	1.2674777163	5.4050130856	9.9657148144
H15	0.7463115878	5.3471984921	9.0077946323
H16	1.9249784348	6.2780627123	9.9371510991
H17	1.9001219537	4.5035994151	10.0676019686
C18	-0.6516732214	4.4058902748	11.0263545591
H19	-1.1775220409	4.4006319990	10.0690838324
H20	-0.1389593124	3.4349292801	11.1473178982
H21	-1.3740813848	4.5085153698	11.8318519296
C22	0.9319537784	5.7233586802	12.3230721680
H23	1.5568985686	4.8656839821	12.6207698200
N27	-0.0925280010	5.9429149634	13.4410191467
O29	0.2072392914	7.0763781905	14.0534183447
O30	-0.6323832774	4.9886311509	14.0371380053

TS14: E= -551.74512828284

N1	2.9544559071	7.1208163907	13.5322750922
C2	3.4630451286	8.4846249224	13.4216412918
H3	2.7617199700	9.2381669829	13.8131732572
H4	3.6712161385	8.7200969697	12.3747574050
H5	4.4004745755	8.5649890487	13.9779407983
C6	2.8051854880	6.7192532559	14.9304813122
H7	2.1418699353	7.3857975553	15.5012768817
H8	3.7903596554	6.7262425275	15.4053009968
H9	2.3987903094	5.7106432579	14.9987332728
C10	1.8234113373	6.8746248596	12.6669036671
H11	2.0892369144	7.3075114321	11.6928700175
N13	0.9140538539	4.8958438182	11.4243109686
C14	0.8135632680	3.4505079885	11.2914625991
H15	0.7040921968	3.1868475549	10.2368975536
H16	1.7190523534	2.9793470828	11.6750923463
H17	-0.0512648799	3.0504381122	11.8398744034
C18	-0.1425878219	5.6382833815	10.7429392002
H19	-0.1296536616	5.3928698723	9.6779362346
H20	-1.1286150183	5.3758632059	11.1501736081
H21	-0.0072838788	6.7078401296	10.8772357327
C22	1.5534067305	5.3981527626	12.5223790682
H23	2.2561477158	4.7138645170	12.9808698184
N27	-0.0858683547	6.6685840111	14.0526635468
O29	0.5970954571	7.5544760403	13.0023137395
O30	-1.2369457318	6.8866348110	14.0693197545

TS15: E= -551.75339614450

N1	2.9359269587	7.1290097447	13.3655730163
C2	3.5204092536	8.4493486425	13.1374899600
H3	2.8822564490	9.2708630239	13.5008785352
H4	3.6980871179	8.5972382003	12.0690875919
H5	4.4846149229	8.5117509828	13.6484523759
C6	2.7759587189	6.8720102420	14.7982453514
H7	2.1056001189	7.5929441278	15.2863125371
H8	3.7573881499	6.9204091990	15.2765991793
H9	2.3701337798	5.8737325555	14.9698520789
C10	1.7170420264	6.9336127110	12.5887199394
H11	1.9333535284	7.3329494510	11.5887751462
N13	0.8770815067	4.9288617206	11.3322485879
C14	0.7722820942	3.4844813977	11.1645447792
H15	0.9448060674	3.2231607422	10.1170043929
H16	1.5259301944	2.9858758982	11.7741419350
H17	-0.2201675729	3.1202786065	11.4557816422
C18	0.0391540684	5.7288311733	10.4372034156
H19	0.4848683802	5.7785717309	9.4382051661
H20	-0.9524088882	5.2732602380	10.3582495215
H21	-0.0882871677	6.7304316884	10.8425532314
C22	1.3639912471	5.4447436622	12.4787122539
H23	1.9576681623	4.7385269538	13.0498024534
N27	-0.0412625559	5.9734587175	13.6360196060
O29	0.5380725169	7.4946686708	13.0831695720



O30	-1.1671758233	5.7584349209	13.3330891497
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TS16: E=-551.73866104666

N1	2.5351087962	7.3964927770	13.5296842791
C2	3.9158556403	7.4659519645	13.0967395313
H3	4.1947086229	8.4634404153	12.7152005690
H4	4.1015658824	6.7406003913	12.2992056149
H5	4.5842898826	7.2251894962	13.9281067132
C6	2.1975933518	8.2359120683	14.6642319868
H7	2.3549462146	9.3069277303	14.4530210722
H8	2.8206924972	7.9583403020	15.5192921833
H9	1.1489099767	8.0929995817	14.9110249208
C10	1.5332438633	7.2770908952	12.4776636212
H11	1.9859134058	7.6038189337	11.5139176698
N13	0.7978404901	5.2384465521	11.0448840046
C14	1.1706291754	3.9368769639	10.5164393601
H15	1.1908800232	3.9711206137	9.4224080037
H16	2.1656500420	3.6599834626	10.8686991289
H17	0.4629444204	3.1524610667	10.8204979790
C18	-0.4557923594	5.7867884367	10.5345845059
H19	-0.3770717934	5.9311049516	9.4520123452
H20	-1.2952613621	5.1082279312	10.7337406179
H21	-0.6513288128	6.7419063663	11.0180141477
C22	1.3160058945	5.6712281574	12.2496765034
H23	2.2142312423	5.1116009538	12.5156220001
N27	0.3504306236	5.5261022143	13.5348397889
O29	0.3595010345	7.8122235472	12.7177471098
O30	-0.5734296899	4.8129279164	13.3651196966

TS17: E= -551.74930234622

N1	2.8882662552	7.1652411021	13.3799977590
C2	3.4092129840	8.5214814973	13.2179939406
H3	2.7235938960	9.2950305890	13.5987550372
H4	3.6017118053	8.7213762519	12.1609609961
H5	4.3582802868	8.6126392723	13.7529690465
C6	2.6891289295	6.8611961304	14.7995098022
H7	1.9545022989	7.5235491455	15.2748571722
H8	3.6472330053	6.9509974818	15.3184085595
H9	2.3312272355	5.8373983348	14.9300642404
C10	1.6631859345	6.9475958317	12.5741180814
H11	1.8953157078	7.4332512129	11.5993858735
N13	0.7836544130	4.9346414539	11.4082182784
C14	0.5206454427	3.4941509592	11.3472956360
H15	0.7049482671	3.1287023862	10.3349845860
H16	1.1761998153	2.9732048771	12.0426419838
H17	-0.5201796879	3.3059049296	11.6195513822
C18	0.0146368195	5.7884201902	10.4852769464
H19	0.6143111719	6.0407391397	9.6083865716
H20	-0.8722213419	5.2414051896	10.1699504970
H21	-0.2770013732	6.6834514386	11.0376271640
C22	1.5256242331	5.4575594243	12.3389649928

H23	1.9859469147	4.7619262488	13.0312839777
N27	-0.4932832740	5.5654200826	14.2307745901
O29	0.4721080684	7.3015459858	13.0890928175
O30	-1.4154946852	5.2537228704	13.5925656041

TS18: E= -513.63988290283

C1	-1.5846746182	1.1603468763	-0.2464572339
H2	-0.5836519022	1.4386883920	-0.5667253825
H5	-2.3944905345	1.9104234571	-1.1347645751
H4	-1.8935927471	1.5736743508	0.7134976135
N10	-1.8234768807	-0.2030818361	-0.3637636175
C12	-3.1056567389	-0.7103719857	0.0992461904
H13	-3.3681345836	-0.2270941632	1.0414078403
H14	-3.8960193644	-0.5072967767	-0.6356731471
H15	-3.0409950023	-1.7883914800	0.2612837894
C15	-1.2635428463	-0.8918777868	-1.5323437207
H16	-1.5301330147	-1.9579597814	-1.4279565472
H17	-1.7527834378	-0.5094674111	-2.4366831896
N26	-3.7379256228	2.1529450407	-2.7403397208
O27	-3.0263694957	2.7106477814	-1.8008165417
O28	-3.6934034108	0.9465527743	-2.8241342895
N16	0.1625626030	-0.6778780530	-1.6378954440
C18	0.9183725831	-1.4335873967	-0.6459323739
H19	0.5313149380	-1.2175365497	0.3511637566
H20	0.8640464646	-2.5251081503	-0.8117689589
H21	1.9684656633	-1.1348976972	-0.6766279347
C21	0.6622871929	-0.8811794431	-2.9919965192
H22	1.7179987874	-0.6035186133	-3.0324949970
H23	0.5743683446	-1.9270777878	-3.3374160764
H24	0.1170168680	-0.2422450331	-3.6896817497

TS19: E= -513.63956893312

C1	-1.5421964319	1.0995046221	-0.1072008067
H2	-0.5315473452	1.4705051808	-0.3044505537
H5	-2.2337919777	1.8374475161	-1.0815756141
N10	-1.6249901827	-0.2707722039	-0.4522082776
C12	-2.7195239507	-1.0759240729	0.0569032385
H13	-2.8510418192	-0.8642796197	1.1177051299
H14	-3.6582005466	-0.8721918310	-0.4769605307
H15	-2.4673954529	-2.1313757713	-0.0696568343
C15	-1.1749275832	-0.6088163843	-1.7925040214
H16	-0.9063249508	-1.6671893827	-1.8289433544
H17	-1.9538484659	-0.4179782292	-2.5430100805
H18	-0.2936510501	-0.0159894530	-2.0461085893
N26	-3.8030830646	2.1635320481	-2.4718850924
O27	-2.7137952370	2.6189123682	-1.9084768715
O28	-4.1773684795	1.0661126986	-2.1252088093
N16	-2.0347026163	1.4759979827	1.1720949526
C18	-3.4265759667	1.9299778713	1.2398416865
H19	-4.0569478306	1.3127731120	0.6018192421
H20	-3.7859718587	1.8487016847	2.2691520694

H21	-3.5362880116	2.9746650842	0.9129012588
C21	-1.1334693155	2.3120780797	1.9554842333
H22	-1.5181540301	2.3985726345	2.9750185730
H23	-0.1456575867	1.8514147617	2.0070227130
H24	-1.0296549036	3.3311839177	1.5473573726

TS20: E= -513.03000650139

C1	3.3468245816	-3.4371612714	-2.6347048564
H2	3.0558292882	-3.5988946196	-1.5967037876
H3	4.4284201077	-3.5718192154	-2.7020668640
N4	2.6836928418	-4.4062839863	-3.5014565674
C5	1.2338900882	-4.3593506545	-3.3978678799
H6	0.8223788387	-4.9170056684	-4.2503088338
C7	3.1343375113	-4.2885133364	-4.8845233506
H8	2.6861811848	-5.0775024860	-5.4928290989
H9	2.8877409564	-3.3138597034	-5.3431860409
H10	4.2190608362	-4.4110540954	-4.9211990780
H11	3.1113661078	-2.3919586115	-2.9045874598
N12	0.7355191603	-4.9433789477	-2.1488611076
C13	0.5418909520	-4.0224088180	-0.5329081109
H14	1.5398074314	-4.1639058125	-0.0733633201
H15	0.4468670915	-3.0366510678	-1.0303311362
C16	1.0224015074	-6.3499201394	-1.9592180354
H17	0.7564749304	-6.6192295700	-0.9356916471
H18	0.4301906026	-6.9719248451	-2.6454994617
H19	2.0808304586	-6.5309039132	-2.1515529187
H20	0.8382112467	-3.3297682076	-3.4476807794
N21	-1.0400718037	-4.7481834684	-2.2577239310
O22	-1.5682170614	-5.7444201561	-2.4647978274
O23	-0.4576577694	-4.5872419519	-0.0311955973

TS21: E= -513.01578855432

N1	0.1651061125	1.7099943038	0.9732167110
C2	-0.5967797762	2.3516961472	2.1520528231
H4	-1.4363390138	2.8974495845	1.6735603738
H5	0.0982815892	3.0943355136	2.5759355920
C6	1.5022406807	1.2351756786	1.3051161977
H7	1.4942331102	0.5305993962	2.1412014277
H8	2.0962425220	2.1034708350	1.5998869660
H9	1.9644970679	0.7759148146	0.4313871817
C10	-0.6518668596	1.0621102308	0.1173157013
H11	-1.4301637678	1.6850039012	-0.3226684788
H12	-1.8143190752	0.5673463057	1.2055850574
N13	-0.2908534792	-0.0344687344	-0.6254829932
C14	0.1568126413	-1.2630469303	0.0429145651
H15	1.0209961142	-1.6887975620	-0.4739846889
H16	0.4148318973	-1.0641374274	1.0788467780
H17	-0.6530314084	-2.0012262532	0.0432240308
C18	-1.0332326026	-0.2728825987	-1.8592187336
H19	-0.4342030467	-0.9037183089	-2.5196424304
H20	-1.9900143832	-0.7811530643	-1.6732754506

H21	-1.2207930786	0.6691865291	-2.3744179002
N24	-2.4691482688	0.5006575041	2.1542812995
O25	-0.9536415863	1.3999338749	3.0074162347
O26	-2.5558870761	-0.6256784110	2.5397405829

TS22: E= -513.05160932644

C1	4.0899106372	-4.7392115593	-4.3520959494
H2	4.5783028726	-3.9980689358	-3.7221286496
H3	4.4176229298	-5.7439938226	-4.0460341844
N4	2.6583807112	-4.5494564720	-4.2396453205
C5	2.1130870295	-3.7799822860	-3.2010656857
H8	1.0996219637	-3.4436245113	-3.4866133801
C9	1.8029397746	-5.2711941132	-5.1515249777
H10	0.7788069801	-4.8980701958	-5.0676915662
H11	2.1325547119	-5.1203296621	-6.1867263405
H12	1.7819774011	-6.3561839314	-4.9671075170
H21	4.4065092549	-4.5857794020	-5.3906071116
N16	1.6978357874	-4.7936828226	-1.8230772639
C18	0.7004697222	-4.2014428923	-0.9648541797
H19	0.5946932152	-3.1435058355	-1.2124665504
H20	-0.2672879441	-4.7038494182	-1.0691405176
H22	1.0083083457	-4.2638076331	0.0906756401
C21	1.7056025371	-6.2415688275	-1.8771474854
H23	1.8883550820	-6.6701262905	-0.8823983258
H24	0.7494952350	-6.6353150822	-2.2446939963
H25	2.4996257455	-6.5716951682	-2.5468545518
O21	2.8804521338	-2.9209313377	-2.5956057541
N22	3.3869304356	-4.2360795117	-1.1423971325
O23	3.2841803163	-3.7590066146	-0.1053679370

TMEDA+2HNO<sub>3</sub>: E= -909.82322501599

C1	-0.7210625889	-0.2328964405	0.5118038193
H2	-1.2982649035	0.2063931782	1.3307188677
H3	-0.0040538952	-0.9226531694	0.9603271754
C4	0.0083233998	0.8697318846	-0.2773942446
H5	0.5436168533	0.4435343506	-1.1276664444
H6	-0.7123770769	1.5875606533	-0.6799508661
N7	1.0041030577	1.6524739798	0.4892625740
N8	-1.6621121426	-1.0645764129	-0.2722564375
C9	-2.8194724011	-0.3214461790	-0.7931091456
H10	-3.2843220282	0.2446778320	0.0167688135
H11	-2.5559563191	0.3699176085	-1.6036042374
H12	-3.5545741102	-1.0313926430	-1.1780591723
C13	-1.0094060066	-1.8698373083	-1.3184936770
H14	-1.7374753422	-2.5761543566	-1.7231030416
H15	-0.6236531489	-1.2639088023	-2.1472638190
H16	-0.1934752013	-2.4391546433	-0.8730565136
C17	0.4198445946	2.4606623018	1.5702836931
H18	-0.4106845318	3.0505961632	1.1770403231
H19	0.0583741381	1.8552319500	2.4111727482
H20	1.1777554666	3.1495982161	1.9491087805

C21	2.1505678136	0.8548620099	0.9568042866
H22	2.9114243870	1.5316412190	1.3515048563
H23	1.8832034580	0.1427544816	1.7469098779
H24	2.5790018515	0.3166897506	0.1111593259
O25	1.9499107914	3.4153276878	-1.2083328247
N26	2.5440777797	2.8033999841	-2.2750325050
O27	3.0114424471	3.5409338961	-3.1020763923
O28	2.5433966350	1.5786219346	-2.2883566832
H29	1.5992939414	2.6609039348	-0.5689996636
O30	-2.6860906261	-2.7786042341	1.4319540890
N31	-1.7114627994	-3.5474268250	2.0014475129
O32	-2.0954594246	-4.3726179579	2.7876750982
O33	-0.5555043350	-3.3257947242	1.6628184648
H34	-2.2163602675	-2.1163470291	0.7681055618

TS23: E= -1114.92388793473

N1	0.5797458094	1.5417183299	0.5272205926
C2	0.1311598820	2.9425141785	0.6008501423
H3	-0.7216013744	3.0333917593	1.2823065091
H4	-0.1623260634	3.2824722237	-0.3936732619
H5	0.9541149319	3.5622082916	0.9559178945
C6	1.2775838816	1.0881300767	1.6627793885
H7	0.4896727809	1.0859670976	2.8482162729
H8	2.0829634662	1.7566784806	1.9616297629
H9	1.5733191446	0.0421685342	1.6154240083
C10	-0.4346693653	0.6233070450	-0.0327086311
H11	-1.0455227237	1.2111005658	-0.7180289360
H12	-1.0902202154	0.2701381394	0.7717535878
N13	-0.7717217971	-1.6043559484	-1.1273835135
C14	-0.0844199716	-2.7981024734	-1.6506063352
H15	0.4479361134	-2.5864469948	-2.5885072216
H16	0.6344672776	-3.1586895343	-0.9123104755
H17	-0.8224323850	-3.5810442856	-1.8247732961
C18	-1.7916558404	-1.1413736232	-2.0842436022
H19	-1.3391636189	-0.8027060486	-3.0276569130
H20	-2.4770205382	-1.9632728148	-2.2874540432
H21	-2.3721170345	-0.3239310914	-1.6555751150
C22	0.2048594781	-0.5561722689	-0.7785901442
H23	0.9597757194	-1.0245816099	-0.1430302514
H24	0.7215792159	-0.1932624872	-1.6804073530
N25	3.6431978624	2.6523875696	-0.9960188530
O26	3.4997589843	3.1299584204	0.1128174672
O27	4.5362588609	2.8092722203	-1.7761060152
O28	2.6318587452	1.7986096387	-1.4397691043
H29	1.9760710841	1.7494027304	-0.6930460509
N30	-2.8993432561	-3.3549555605	0.8550173143
O31	-3.0739080821	-3.6550018218	-0.3173885442
O32	-3.4752954702	-3.7843639779	1.8175687120
O33	-1.9309142253	-2.4185306657	1.1185391539
H34	-1.5309330461	-2.1317288259	0.2066674553
N36	-1.2655825247	1.2687124354	3.9528113798

O37	-1.7972050688	1.5016779023	2.8988657859
O38	0.0157373492	1.0345931157	3.9475450120

TS24: E= -1114.92588740551

N1	0.9210182071	1.4680716474	0.8836915380
C2	0.1849242698	2.7163352605	1.1434317235
H3	-0.1711080842	2.7428676911	2.1784859138
H4	-0.6672083713	2.7818977670	0.4656051251
H5	0.8495464854	3.5604867129	0.9591077162
C6	2.1472446683	1.3622317681	1.6910582092
H7	1.8963718590	1.3357775241	2.7580172523
H8	2.7787112711	2.2265194162	1.4872650550
H9	2.6978079943	0.4591870983	1.4284999435
C10	0.1170335431	0.3101855262	0.7898788222
H11	-0.8252014259	0.5228879642	0.2856610469
H12	-0.3481463530	-0.0693169645	2.0600881090
N13	-0.1473551407	-1.8261419678	-0.4471949898
C14	0.2273903648	-3.2496612009	-0.3831863659
H15	1.2209964845	-3.4325150154	-0.8167368293
H16	0.2270930923	-3.5790171311	0.6573177008
H17	-0.5134782895	-3.8325198482	-0.9297111313
C18	-0.2368402903	-1.3762311041	-1.8488436893
H19	0.7186731978	-1.5057448770	-2.3754606224
H20	-1.0118845774	-1.9501066565	-2.3561824305
H21	-0.5081632147	-0.3200773648	-1.8883316803
C22	0.7840403503	-0.9871765970	0.3306390872
H23	1.1096671333	-1.5668776199	1.1980018618
H24	1.6855230136	-0.7672612419	-0.2638494533
N25	2.6647608326	2.8443004904	-1.8933121470
O26	2.8665547012	3.4906328046	-0.8827801311
O27	3.0957071781	3.0151992354	-2.9961614010
O28	1.8153660354	1.7458639092	-1.7674661290
H29	1.5404259967	1.7271340109	-0.8066101947
N30	-3.5239395323	-2.3165945735	-0.2949912684
O31	-3.0282113178	-3.0560511818	-1.1319929725
O32	-4.6864474312	-2.1880971924	-0.0227464882
O33	-2.6627197935	-1.5296932422	0.4308980607
H34	-1.7091625302	-1.7278609827	0.0937348927
N36	-0.7050416560	0.0483769758	4.1326224513
O37	-0.7028752645	-0.6775570231	3.0516897289
O38	-0.3363643736	1.1900630376	4.0440834956

TMMDA+2HNO<sub>3</sub>: E= -870.50182147672

N1	1.0677438638	0.6338197365	-1.0736155167
C2	1.7982283786	-0.3259128699	-0.2238222568
H3	2.2415662951	-1.1365415778	-0.8191620876
H4	1.1319851460	-0.7645457461	0.5158339473
H5	2.5882062757	0.2099727095	0.3005853227
C6	2.0016947038	1.3015810059	-2.0028550720
H7	2.4854940939	0.5836009397	-2.6800188444
H8	2.7672557998	1.8152816709	-1.4229211133

H9	1.4630601407	2.0403204892	-2.5997463006
N10	-1.0677438638	-0.6338197365	-1.0736155167
C11	-2.0016947038	-1.3015810059	-2.0028550720
H12	-2.4854940939	-0.5836009397	-2.6800188444
H13	-1.4630601407	-2.0403204892	-2.5997463006
H14	-2.7672557998	-1.8152816709	-1.4229211133
C15	-1.7982283786	0.3259128699	-0.2238222568
H16	-2.2415662951	1.1365415778	-0.8191620876
H17	-2.5882062757	-0.2099727095	0.3005853227
H18	-1.1319851460	0.7645457461	0.5158339473
C19	0.0000000000	0.0000000000	-1.8614089808
H20	0.4267365422	-0.7800637010	-2.5098459758
H21	-0.4267365422	0.7800637010	-2.5098459758
H26	0.6356216390	1.9397288994	-0.1326195707
N27	-1.3677109952	-3.3026624508	1.0629636402
O28	-0.3008735519	-2.7714641550	0.3735946812
O29	-1.1157995638	-4.2797239190	1.7133424372
O30	-2.4423369985	-2.7355650719	0.9456383823
H31	-0.6356216390	-1.9397288994	-0.1326195707
N37	1.3677109952	3.3026624508	1.0629636402
O38	2.4423369985	2.7355650719	0.9456383823
O39	1.1157995638	4.2797239190	1.7133424372
O40	0.3008735519	2.7714641550	0.3735946812

TS25: E= -1075.59866551431

N1	0.2142630567	0.4481803782	1.2924377431
C2	-0.4087577949	-0.4642694860	2.2671859338
H3	0.2271998847	-1.3332531895	2.4812581095
H4	-1.3718492231	-0.8133534590	1.8966164769
H5	-0.5880839115	0.0811788772	3.1946525964
C6	1.4392042711	1.0518295849	1.8570487645
H7	2.2064704965	0.2950446602	2.0711849207
H8	1.1866297447	1.5627293683	2.7871380937
H9	1.8367451855	1.7861602710	1.1566808182
N10	-0.5883655750	-0.7110863696	-0.7376008441
C11	-0.2356169735	-1.6336608944	-1.7421209973
H12	0.5259056020	-1.0893229853	-2.8061076497
H13	0.4268431295	-2.4230063882	-1.3904480724
H14	-1.0940435521	-1.9981282268	-2.3051466707
C15	-1.5499170087	0.3234743965	-1.1529293483
H16	-1.0454689241	1.0895585390	-1.7525602075
H17	-2.3359771995	-0.1430549126	-1.7469064166
H18	-2.0020706671	0.7914008209	-0.2810305581
C19	0.5654815290	-0.2111713100	0.0284325020
H20	1.2206508319	-1.0730302918	0.2136260557
H21	1.1007400587	0.5173337610	-0.5900289884
H26	-0.7560544632	1.8139156925	1.2328385181
N27	-1.4527910203	-3.8754833092	0.9519361403
O28	-2.2556541646	-2.8367406774	0.4642803277
O29	-2.0611766361	-4.8243101059	1.3484056033
O30	-0.2519864236	-3.6890016390	0.9162600191

H31	-1.6191099567	-2.1442938407	0.1600860269
N37	-0.8906909705	3.6466035134	0.6149567814
O38	0.0948508009	3.4044379398	-0.0607040224
O39	-1.5019952129	4.6756333689	0.6980828604
O40	-1.3811899861	2.6113260458	1.3887271194
N33	1.5783738954	0.3815557266	-3.8416590940
O34	1.1427423785	-0.8448462038	-3.8093932542
O35	1.3284211313	1.0902346750	-2.9021102995

TS26: E= -1075.59976983060

N1	0.2610055045	0.4101855597	0.9758110733
C2	-0.5308361893	-0.3121226856	2.0017126916
H3	-0.0086315653	-1.2114614062	2.3510048986
H4	-1.5031136677	-0.5969573843	1.6028203591
H5	-0.6943370021	0.3566127937	2.8480949135
C6	1.5311960745	0.8928292976	1.5603090408
H7	2.1689274418	0.0599037087	1.8862415190
H8	1.3033832224	1.5159805915	2.4259993610
H9	2.0681320286	1.4935271256	0.8285029108
N10	-0.5901969981	-0.8303786147	-0.9435676539
C11	-0.2166177590	-1.6693009390	-2.0979313273
H12	0.2124382704	-1.0556034793	-2.8967152489
H13	0.5018056067	-2.4255404487	-1.7820006904
H14	-1.1088945548	-2.1697171592	-2.4766900227
C15	-1.6154527827	0.1693925896	-1.2916395924
H16	-1.2036705882	0.9028839203	-1.9933997449
H17	-2.4555560643	-0.3449130403	-1.7597839577
H18	-1.9736969109	0.6806820999	-0.4014289129
C19	0.5287661255	-0.3832360301	-0.2023678165
H20	1.2269202411	-1.2116253250	-0.0219882985
H21	1.3755228553	0.3923749919	-1.0335864710
H26	-0.5729098223	1.9017379821	0.8193553902
N27	-1.1978408118	-3.8992271437	0.7822404237
O28	-2.0601098701	-2.9216536088	0.2866932857
O29	-1.7444894560	-4.8658918214	1.2254364540
O30	-0.0071747984	-3.6576316005	0.7082775956
H31	-1.4663721693	-2.1929768158	-0.0486421858
N37	-0.6281884691	3.6894841215	0.0896171227
O38	0.2818707842	3.3316161407	-0.6348369935
O39	-1.1610823747	4.7620109230	0.1500603549
O40	-1.1289526608	2.7398062559	0.9669476219
N33	2.0032704386	1.4749618137	-2.7395071499
O34	0.9084728268	1.2701512141	-3.1874321716
O35	2.2913125117	0.9750185278	-1.5702159247